Delaware Department of Natural Resources and Environmental Control

# **APPENDICES**

# MURDERKILL RIVER WATERSHED TMDL MODEL DEVELOPMENT AND CALIBRATION

Prepared by:

HDR|HydroQual

KCDW - 178287 **December**, **2013** 



# **APPENDIX 1**

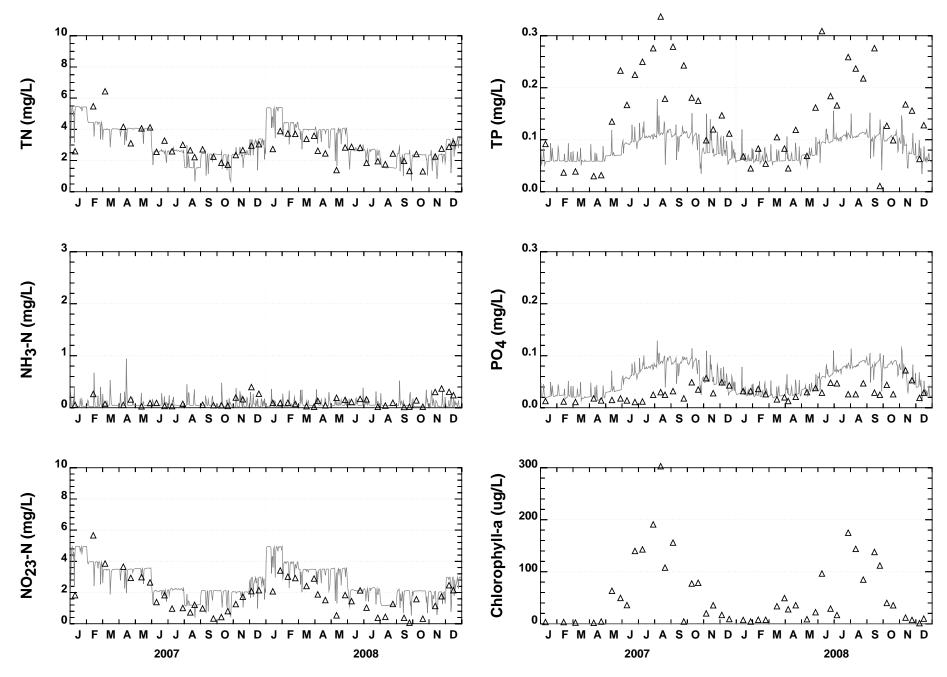
# HSPF MODEL SUBWATERSHED LAND USE

#### Murderkill River Watershed HSPF Subwatershed Land Use (Areas in acres)

	Agricultural	CAFO	Forest	Open Water	Pasture or		Residential		Streets or	Transitional		Urban		Wetlands		Total	
					Rangeland				Parking								
Reach	PERLND	PERLND	PERLND	PERLND	PERLND	IMPLND	PERLND	Total	IMPLND	PERLND	IMPLND	PERLND	Total	PERLND	IMPLND	PERLND	Total
RCHRES 2	2628	0	701	13	7	635	635	1270	24	116	17	17	34	457	676	4574	5250
RCHRES 3	260	0	40	8	5	27	27	54	0	0	0	0	0	25	27	365	392
RCHRES 4	1882	16	216	7	26	552	552	1104	27	44	51	51	102	782	630	3576	4206
RCHRES 5	833	0	130	40	0	122	122	244	0	2	13	13	26	54	135	1194	1329
RCHRES 6	201	0	77	13	0	27	27	54	0	0	0	0	0	24	27	342	369
RCHRES 7	1829	21	259	3	27	203	203	406	23	21	30	30	60	138	256	2531	2787
RCHRES 8	521	0	71	21	13	121	121	242	0	0	0	0	0	28	121	775	896
RCHRES 8	521	0	71	21	13	121	121	242	0	0	0	0	0	28	121	775	896
RCHRES 9	118	0	89	12	0	26	26	52	0	0	0	0	0	11	26	256	282
RCHRES 10	264	0	196	19	0	7	7	14	0	0	0	0	0	41	7	527	534
RCHRES 11	952	0	264	42	0	31	31	62	16	0	11	11	22	211	58	1511	1569
RCHRES 12	1623	21	341	4	39	254	254	508	13	32	26	26	52	595	293	2935	3228
RCHRES 13	3267	12	786	19	22	143	143	286	22	12	6	6	12	995	171	5262	5433
RCHRES 14	1120	19	219	2	27	26	26	52	14	0	29	29	58	159	69	1601	1670
RCHRES 15	225	2	214	74	3	89	89	178	0	0	0	0	0	51	89	658	747
RCHRES 16	1283	19	345	22	2	58	58	116	14	0	22	22	44	120	94	1871	1965
RCHRES 17	501	0	44	38	0	31	31	62	0	0	0	0	0	9	31	623	654
RCHRES 18	852	0	113	94	0	53	53	106	2	0	0	0	0	105	55	1217	1272
RCHRES 19	1442	25	422	13	14	150	150	300	0	39	1	1	2	98	151	2204	2355
RCHRES 20	1175	0	274	4	6	196	196	392	4	0	68	68	136	166	268	1889	2157
RCHRES 21	783	0	292	19	16	337	337	674	32	14	145	145	290	543	514	2149	2663
RCHRES 22	1	0	2	0	0	0	0	0	0	0	1	1	2	3	1	7	8
RCHRES 23	1607	5	389	35	0	229	229	458	15	116	56	56	112	224	300	2661	2961
RCHRES 24	625	11	141	39	74	67	67	134	0	157	0	0	0	114	67	1228	1295
RCHRES 25	211	0	33	43	0	22	22	44	0	0	0	0	0	6	22	315	337
RCHRES 26	1265	9	267	72	182	104	104	208	0	0	0	0	0	158	104	2057	2161
RCHRES 27	3405	10	434	69	16	152	152	304	10	14	23	23	46	562	185	4685	4870
RCHRES 28	2871	13	504	116	25	95	95	190	57	33	38	38	76	1289	190	4984	5174
TOTAL	31744	183	6863	841	504			7514	273	600			1074	6968			56564

# **APPENDIX 2**

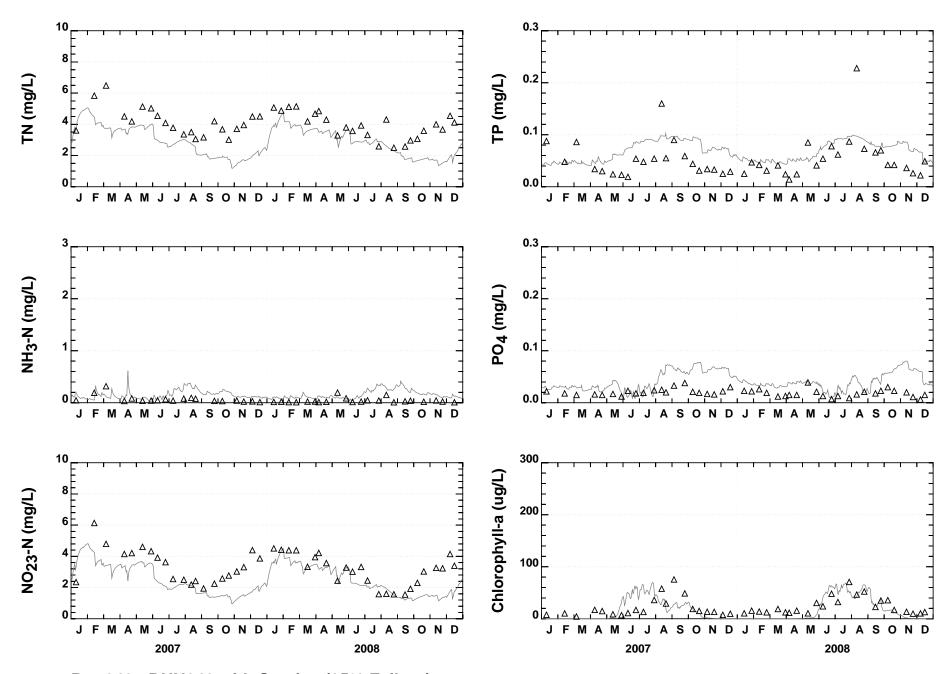
# HSPF MODEL CALIBRATION/VALIDATION FIGURES



Run046 - RUN046 with Septics (25% Failure)

Water Quality Data at Station 206561, Double Run at Barratts Chapel Rd. (Rd. 371)

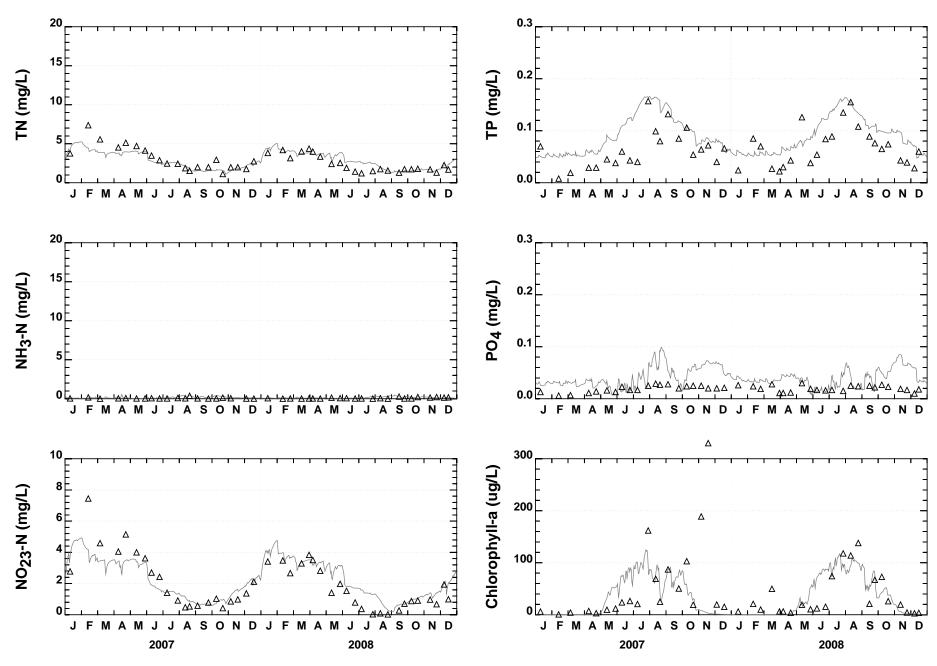
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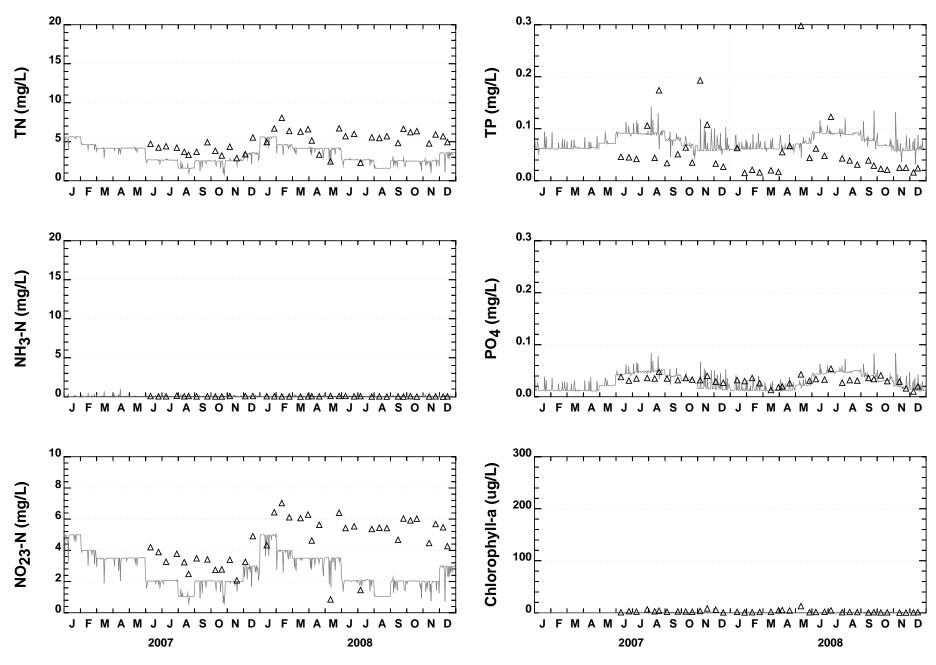
Run046 - RUN046 with Septics (25% Failure)

Water Quality Data at Station 206461, McGinnis Pond at McGinnis Pond Rd. (Rd. 378)

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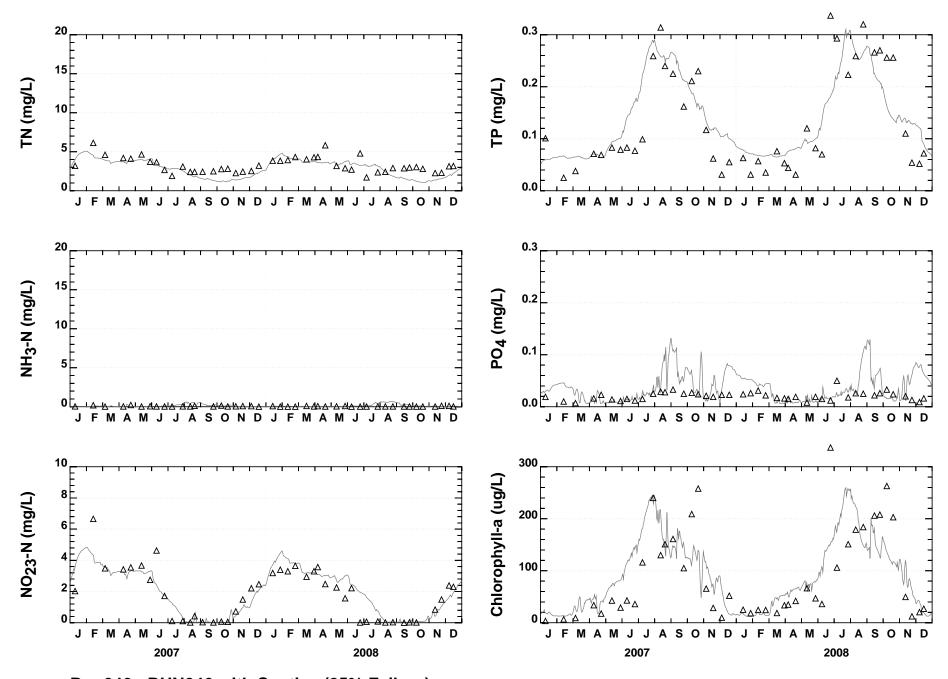


Run046 - RUN046 with Septics (25% Failure)
Water Quality Data at Station 206071, Andrews Lake at Rd. 380 Brdg.
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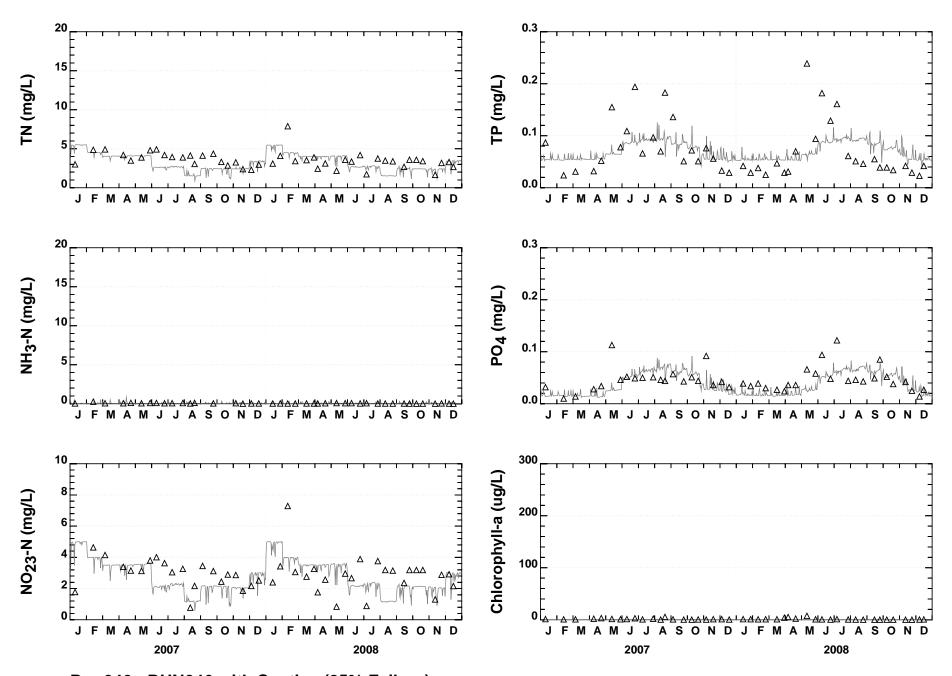


Run046 - RUN046 with Septics (25% Failure)

Water Quality Data at Station 206641, Spring Creek, Pratt Branch at Canterbury Rd.



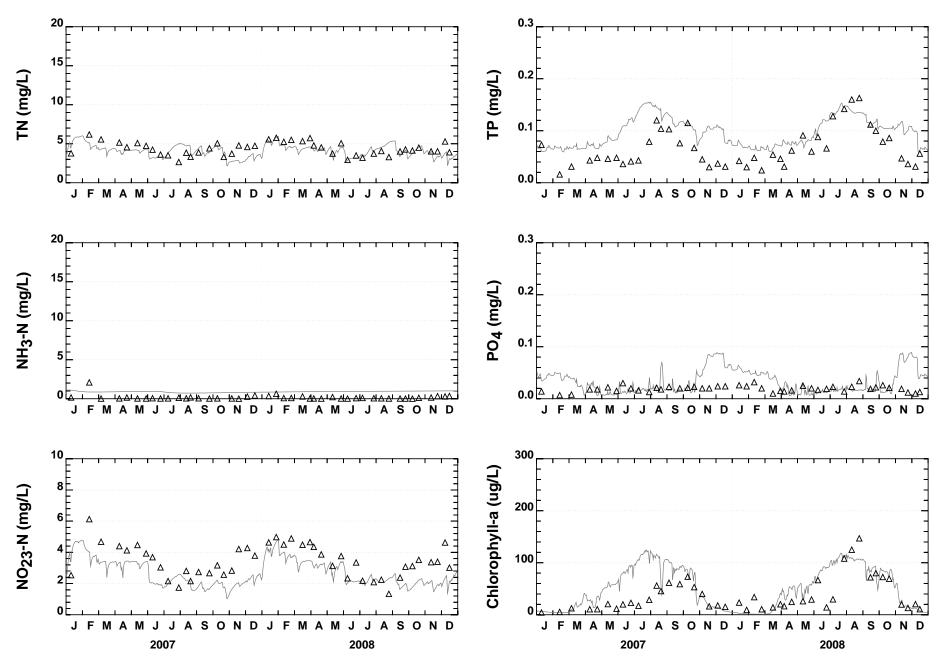
Run046 - RUN046 with Septics (25% Failure) Water Quality Data at Station 206451, Coursey Pond at Canterbury Rd. (Rt. 15) at Rd. 388 Bridge



Run046 - RUN046 with Septics (25% Failure)

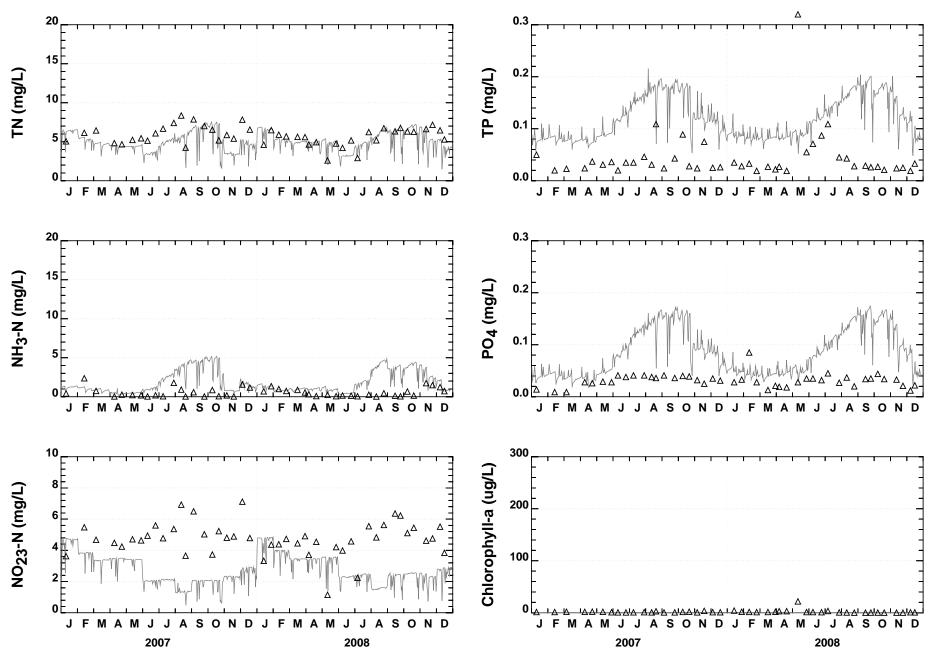
Water Quality Data at Station 206011, Murderkill River at Confluence of Black Swamp Creek

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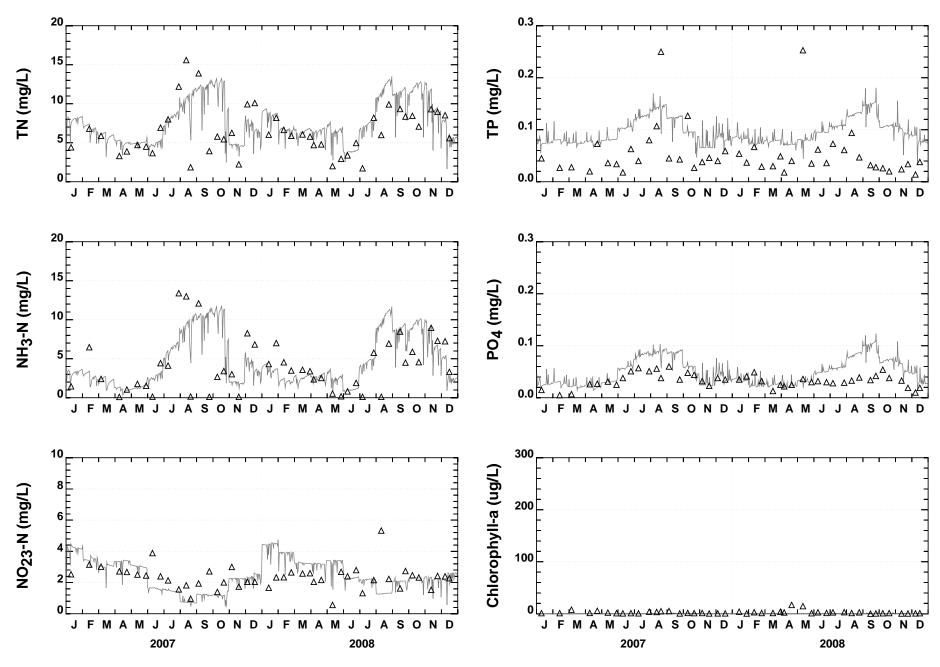


Run046 - RUN046 with Septics (25% Failure)

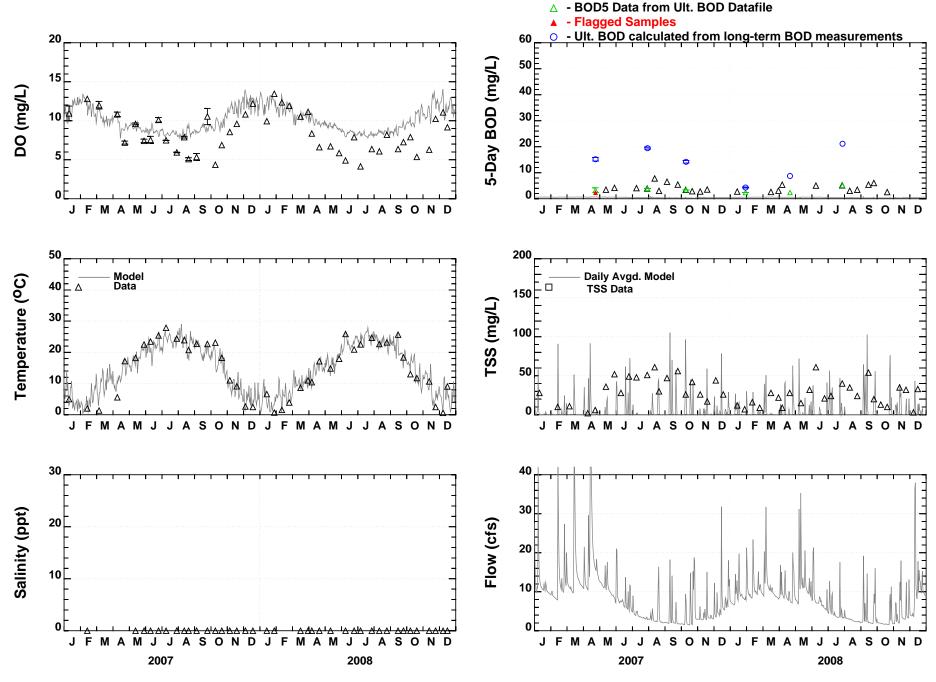
Water Quality Data at Station 206361, McColley Pond at Canterbury Rd. (Rt. 15) near Spillway



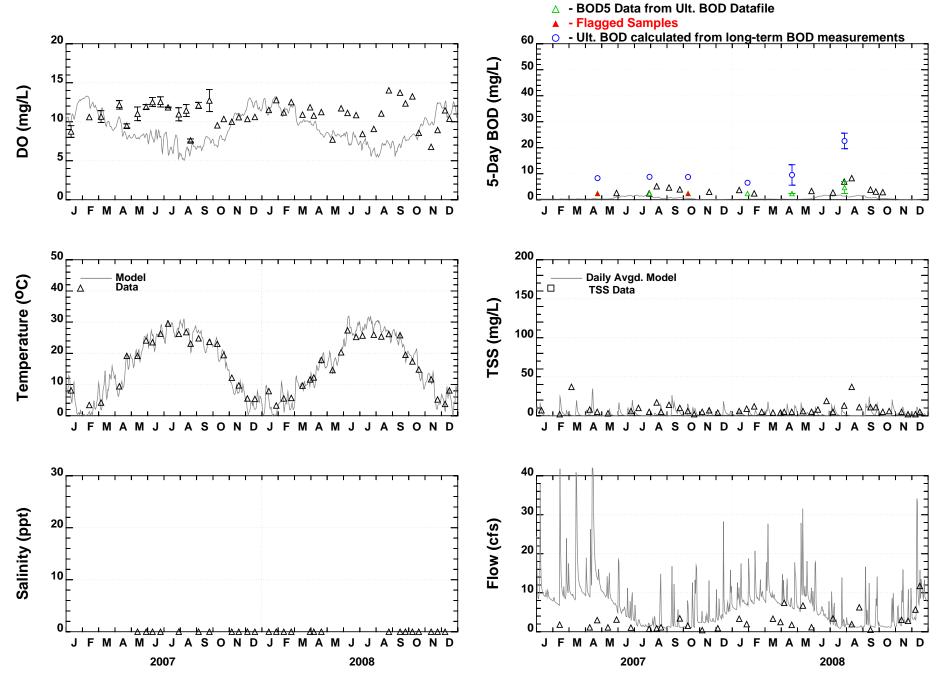
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Run046 - RUN046 with Septics (25% Failure) Water Quality Data at Station 206041, Browns Branch at Milford-Harrington Hwy. (Rt 14)

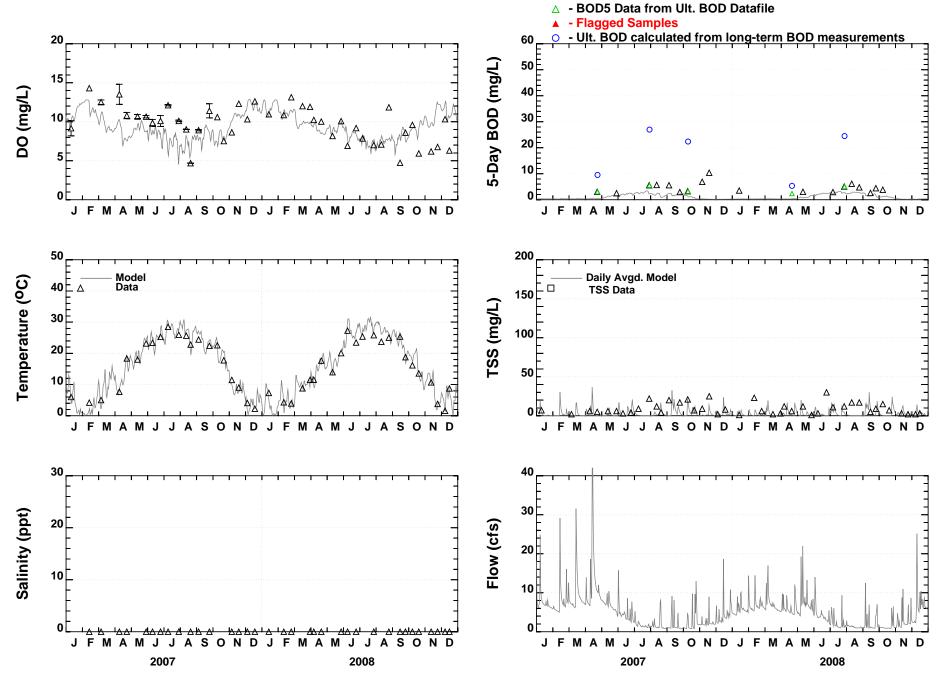


**RUN046 with Septics (25% Failure)** Water Quality Data at Station 206561, Double Run at Barratts Chapel Rd. (Rd. 371)



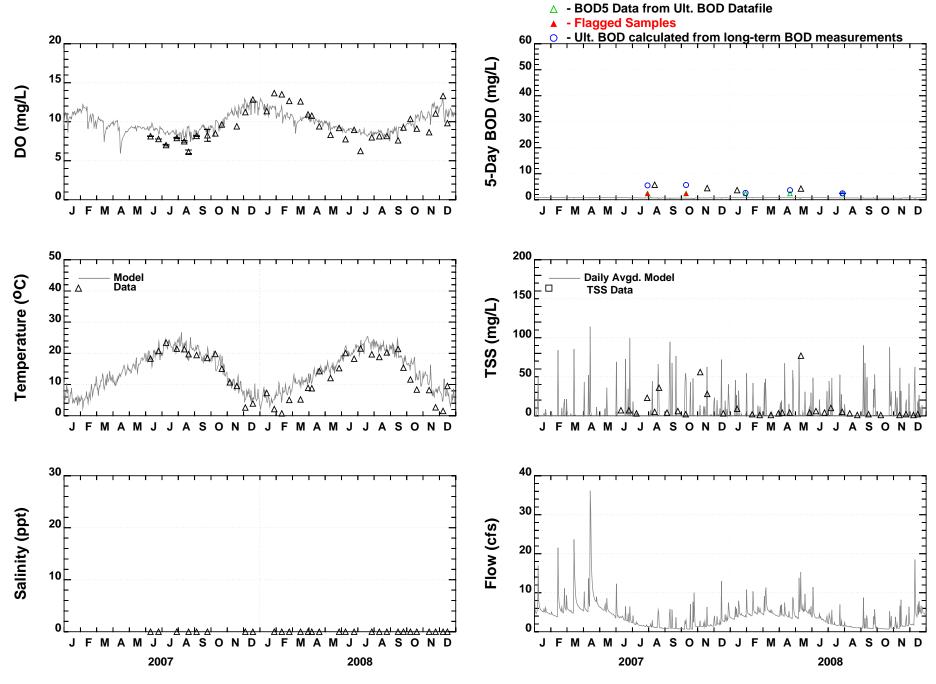
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Water Quality Data at Station 206461, McGinnis Pond at McGinnis Pond Rd. (Rd. 378)



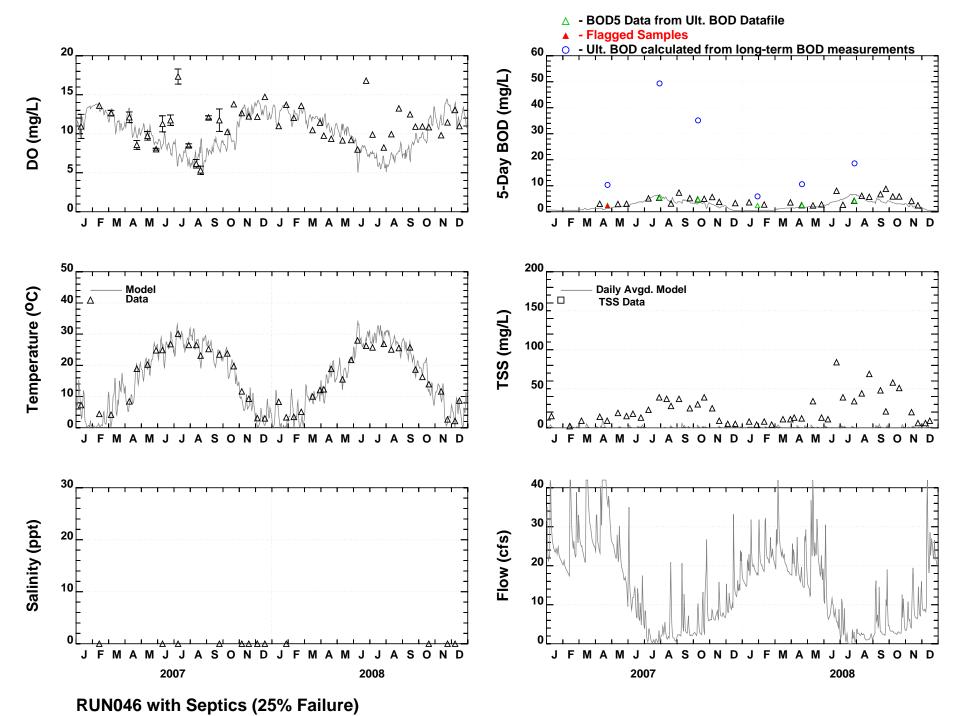
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Water Quality Data at Station 206071, Andrews Lake at Rd. 380 Brdg.



RUN046 with Septics (25% Failure)
Water Quality Data at Station 206644. Spring Creek, Brat

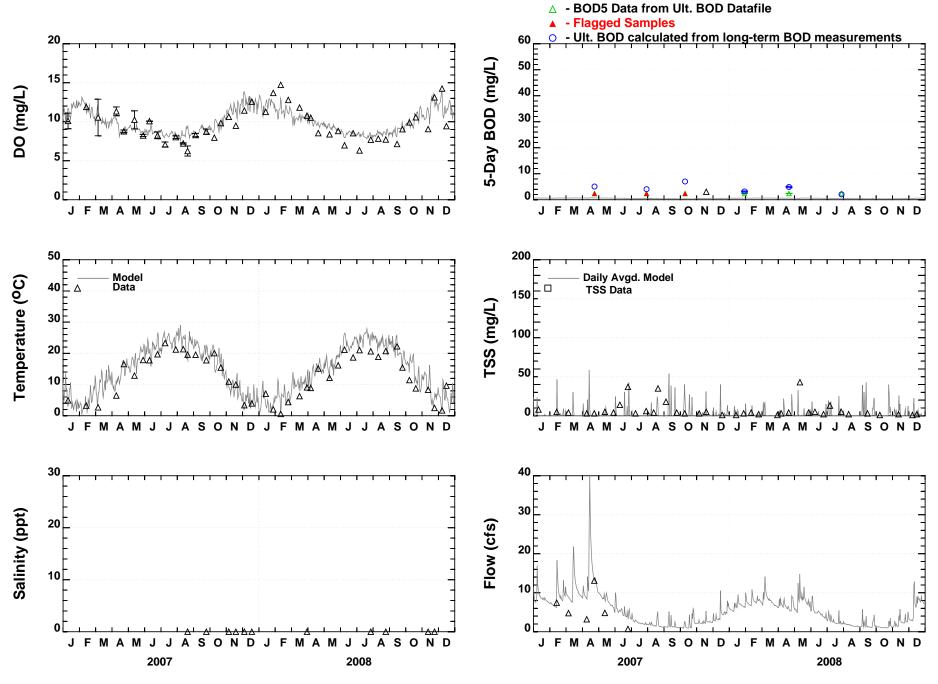
Water Quality Data at Station 206641, Spring Creek, Pratt Branch at Canterbury Rd. /white5/kcdw0014/WQ/DATA/Plot\_LY/ptemp2.gdp (sedplot6p.sh)



Water Quality Data at Station 206451, Coursey Pond at Canterbury Rd. (Rt. 15) at Rd. 388 Bridge

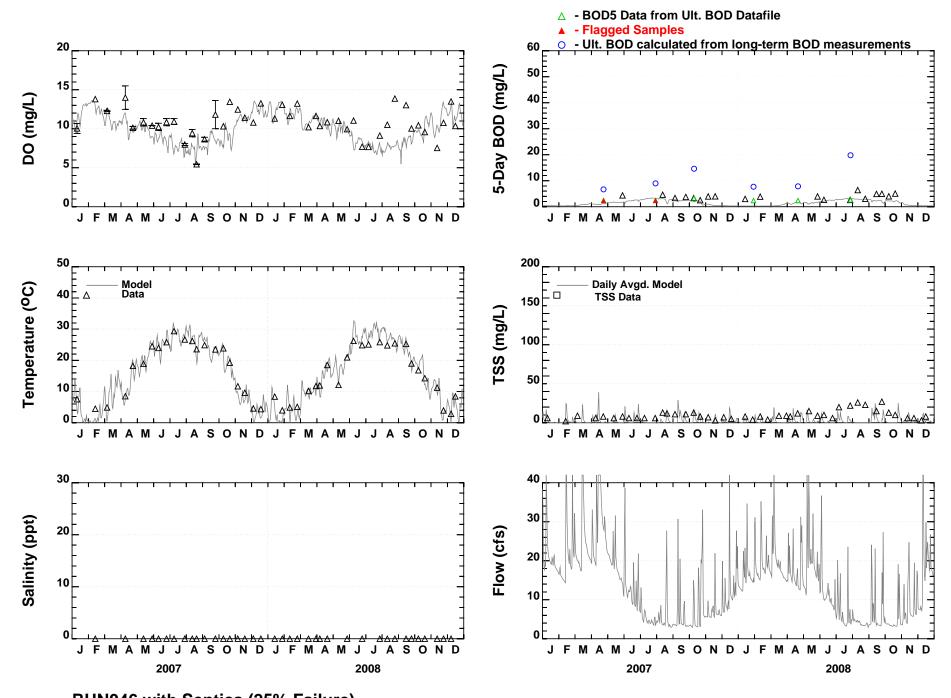
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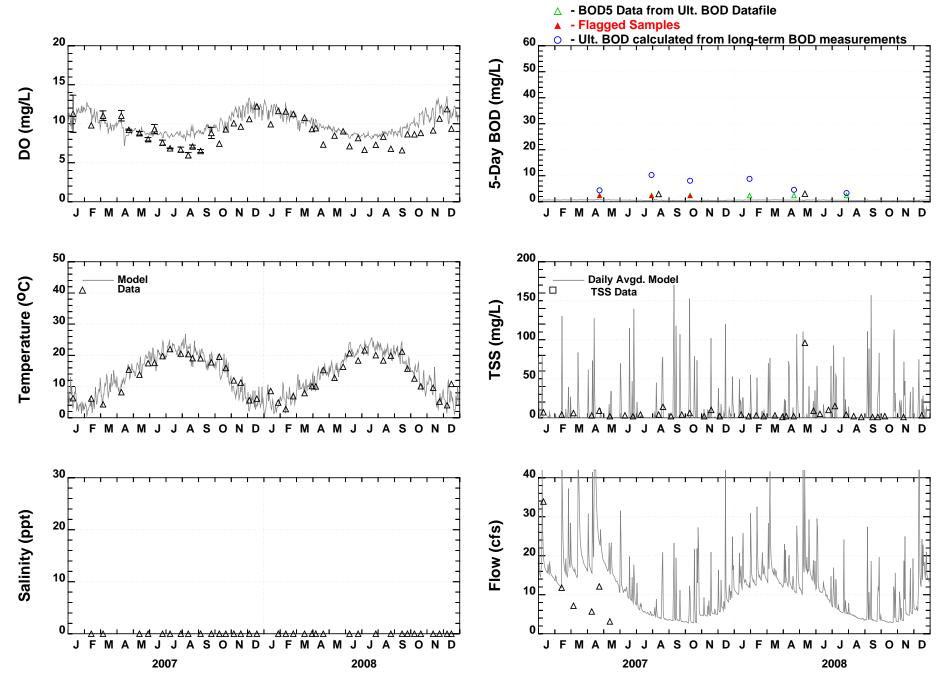


**RUN046 with Septics (25% Failure)** 

Water Quality Data at Station 206011, Murderkill River at Confluence of Black Swamp Creek /white5/kcdw0014/WQ/DATA/Plot\_LY/ptemp2.gdp (sedplot6p.sh)

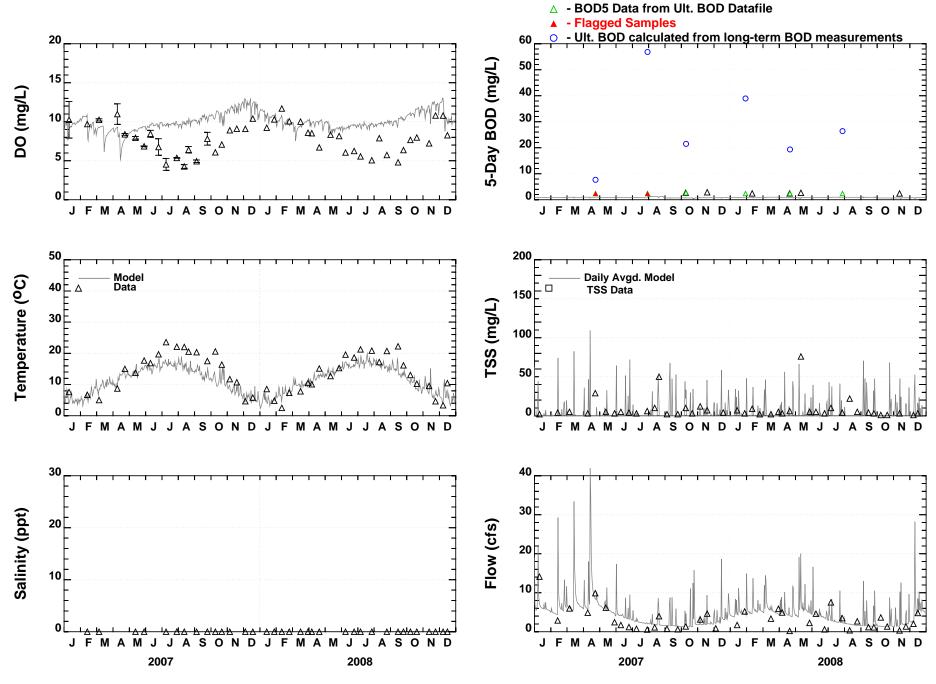


RUN046 with Septics (25% Failure)
Water Quality Data at Station 206361, McColley Pond at Canterbury Rd. (Rt. 15) near Spillway



RUN046 with Septics (25% Failure)

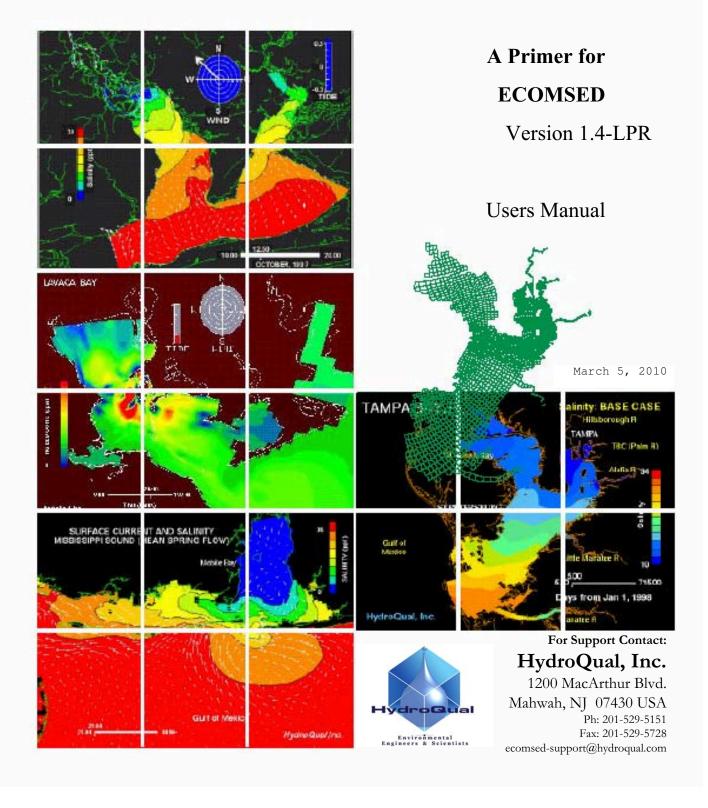
Water Quality Data at Station 206051, Browns Branch at Killens Pond Rd. (Rd. 384)
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#### **PREFACE**

The development of ECOMSED has its origins in the mid 1980's with the creation of the Princeton Ocean Model (Blumberg and Mellor, 1987) and its version for shallow water environments - rivers, bays, estuaries and the coastal ocean and reservoirs and lakes- named ECOM (Blumberg, 1996). In the mid 1990s, concepts for cohesive sediment resuspension, settling and consolidation (Lick, et al., 1984) were incorporated within the ECOM modeling framework. During the last several years, ECOMSED was enhanced to include generalized open boundary conditions, tracers, better bottom shear stresses through a submodel for bottom boundary layer physics, surface wave models, noncohesive sediment transport, and dissolved and sediment-bound tracer capabilities. The code has been reconfigured to be easily ported to almost any computer system, from PCs to workstations to super mainframes. Model performance has been evaluated by appealing to a large series of simple test cases designed to isolate specific processes and by application of the model to many real-world situations. There have been over 350 journal articles written that are based on the use of the various ECOMSED submodels. While there is a real confidence that ECOMSED is "bug free", it remains the user's responsibility to check and recheck their own results via their own test cases and their own comparisons with data.

The ECOMSED system has proven over the years to be quite robust and reliable. A user's guide on the other hand has been elusive. The material presented herein is directed towards the goal of a detailed, well documented manual that hopefully will allow enable an educated user to address real world environmental problems using sophisticated technology with the labor of learning all the details of the model's composition.

Today's version of ECOMSED and this manual have been made possible by the dedicated efforts of Parmeshwar L. Shrestha, B. Nicholas Kim, Quamrul Ahsan and Honghai Li. They have helped conceive, design and implement the model enhancements and worked diligently to debug their (and my) changes. The manual owes its form and content to them. Important contributions to various aspects of ECOMSED have also been made at one time or another by Boris Galperin, H. James Herring, Eugenio Gomez-Reyes, C. Kirk Zeigler, and Richard P. Signell. Finally, the seminal contributions of George L. Mellor must be acknowledged. It was he who first managed to secure funding which made the Princeton Ocean Model a reality.

HydroQual, Inc.



#### 1.0 Introduction

This primer describes the use of a fully integrated three-dimensional hydrodynamic, wave and sediment transport model, ECOMSED. The model is designed to simulate with as much realism as possible time-dependent distributions of water levels, currents, temperature, salinity, tracers, cohesive and noncohesive sediments and waves in marine and freshwater systems. The three ECOMSED sub-models are designed to work in conjunction with one another, with output from one serving as input to another. The same orthogonal curvilinear computational grid structure and underlying numerical solution techniques are utilized for all sub-models. The wave sub-model embedded in ECOMSED utilizes wave parameters to accurately compute the wave-induced bottom friction necessary for calculation of bed shear stresses at the sediment-water interface. ECOMSED uses an orthogonal curvilinear coordinate system, greatly increasing model efficiency in treating irregularly shaped coastlines and in meeting requirements for high resolution at desired locations.

The ECOMSED model is capable of simulating the transport and fate of suspended sediments, dissolved tracers and neutrally-buoyant particles in estuarine and coastal ocean systems. A wide variety of problems concerning water optics and spill tracking can be studied using the model due to the various options built into ECOMSED. Capabilities of the model include: (1) runtime computed (internal) or precomputed (external) hydrodynamics; (2) cohesive and non-cohesive sediment transport; (3) sediment-bound tracer transport (conservative or first-order decay); (4) dissolved tracer transport (conservative or first-order decay); (5) neutrally-buoyant particle tracking; and (6) inclusion of wind wave effects on hydrodynamics and sediment transport. Descriptions of ECOMSED options and capabilities are provided in the following section.

The development of ECOMSED is an ongoing topic of research. The user of this version (1.2) can expect modifications, some of which will be "fixes" to the code and others which will be enhancements to the present water physics and sediment dynamics. Many changes in this primer are planned and some already implemented. Please direct any suggestions and critical comments to ecomsed-support@hydroqual.com. All ideas are welcome and many may find themselves in the next version of this primer.



#### 2.0 ECOMSED Model Features

The ECOMSED is a state-of-the-art hydrodynamic and sediment transport model which realistically computes water circulation, temperature, salinity, and mixing and transport, deposition and resuspension of cohesive and non-cohesive sediments. The complete ECOMSED model consists of several modules. These are hydrodynamic module, sediment transport module, wind induced wave module, heat flux module and particle tracking module. Figure 2.1 illustrates the ECOMSED modeling framework. The ECOMSED is also coupled with HydroQual's state-of-the-art water quality model, RCA by a sophisticated and efficient interface. The modules within the ECOMSED modeling framework are linked internally. These modules can be turned on and off by the users depending upon their needs. The ECOMSED modeling framework also allows for linking each module externally. For example, the hydrodynamic module can be run stand alone and transport information can be saved in a separate file. Then the sediment module can be run stand alone using the previously saved transport information, and so is the water quality module, RCA. The following section describes the various features of ECOMSED in detail.

#### 2.1 Internal/External Hydrodynamics

Hydrodynamic simulations are required to provide advection and dispersion information for the water-borne constituent transport algorithms. ECOMSED can use either internal or external hydrodynamic information. When the internal hydrodynamic option is chosen, the ECOM hydrodynamic model, which is built into ECOMSED, runs in parallel with the sediment and tracer transport algorithms. The external hydrodynamic option of ECOMSED allows the model to use previously-generated hydrodynamic information that has been stored in computer files. Simulation of sediment and tracer transport is accomplished by reading hydrodynamic information from the previously-generated computer files. This method has the advantage of reduced computational times when compared to the internal hydrodynamic option. However, care must be taken when using the external option because the previously-generated transport files required to study a particular aquatic system may be too large to handle. In other words, computer storage requirements could limit the temporal length of simulations to the point that the external option cannot be used effectively for a specific problem.

#### 2.2 Sediment Transport

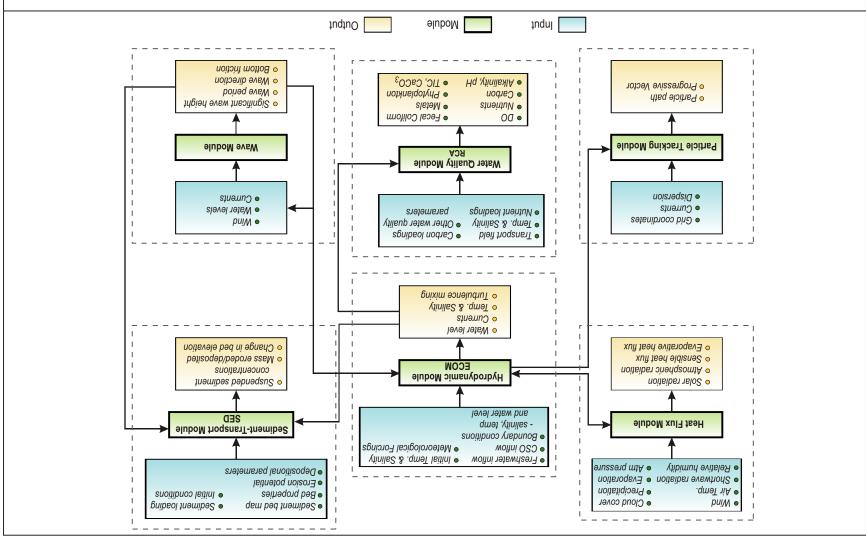
The transport and fate of cohesive and non-cohesive sediments can be simulated with ECOMSED. Resuspension, deposition and transport of cohesive sediments, which are composed of clays, silts and organic material, are simulated using the SED module. The suspended transport of non-cohesive sediments, i.e., fine sands, is calculated using the van Rijn procedure (van Rijn, 1984). The effects of bed armoring due to particle-size heterogeneity can also be included in non-cohesive sediment transport simulations. See Section 6 for a more detailed description of the sediment dynamics included in the cohesive and non-cohesive sediment modules. The sediment transport module can





#### **EICHKE 7-1**

### ECOMSED Modeling Framework



predict temporal and spatial distributions of: (1) suspended sediment concentrations (cohesive and non-cohesive); (2) sediment bed elevation changes; (3) fluxes at the sediment-water interface; and (4) changes in sediment bed composition. The module can accept as input: spatially-variable sediment bed properties and time-variable sediment loading at river discharges and open boundaries.

#### 2.3 Sediment-bound Tracer Transport

The fate of sediments from a particular source, e.g., river discharge or specific sediment bed location, can be determined using ECOMSED. This type of simulation is accomplished by using a sediment-bound tracer, which is analogous to a hydrophobic contaminant, e.g., organic chemical, heavy metal or radionuclide, that adsorbs to fine-grained sediment particles. However, in these simulations the tracer is permanently adsorbed to the sediment particles; actual hydrophobic contaminants are partially soluble and exist in both particulate and dissolved form, with a high percentage of the contaminant being adsorbed to sediment particles.

The transport and fate of sediment-bound tracers can be simulated for both cohesive and non-cohesive sediments. In addition, the tracer can be conservative or be assigned a first-order decay rate, which would approximate a sediment-bound radionuclide. Of particular importance is the use of a sediment bed model that makes it possible to simulate changes in tracer bed concentrations due to deposition and erosion; temporal and spatial (horizontal and vertical) variations in tracer bed concentrations can be predicted. The bed model can also simulate the effects of bioturbation on tracer mixing in the surficial layer of the bed.

#### 2.4 Dissolved Tracer Transport/Pathogen Fate Model

Simulation of the transport of a dissolved tracer and pathogen can be accomplished using ECOMSED, with the tracer being either conservative or having a first-order decay rate depending on the water column temperature, salinity and insolation rates. This type of calculation can be useful for determining the fate of a water-borne contaminant released from a particular location, e.g., river discharge, offshore diffuser or open boundary. Temporally varying tracer concentrations can be specified for all three types of boundary conditions.

#### 2.5 Particle Tracking

This option allows the tracking of discrete particles that can be released into the aquatic system at various locations. These particles are neutrally-buoyant and conservative. A Lagrangian technique is used to advect the particles and a random-walk procedure is employed to simulate the effects of turbulent diffusion. A complete description of the theory and numerical methods used in the particle tracking module can be found in Zhang (1995).

The particle tracking module can be useful for the simulation of oil spills or studying the trajectories of floating objects. Particles can be released from multiple locations at



variable rates. In addition, each released particle has associated with the time and location of its release, which has been helpful information in previous analyses.

#### 2.6 Wind Waves

Resuspension of sediments due to wind-generated waves is an important source of sediment to the water column in many coastal ocean systems. The effects of wind waves on bottom shear stress, which controls sediment resuspension, can be accounted for by ECOMSED. Temporally and spatially variable wind wave parameters, i.e., mean period, significant wave height and direction, can be calculated using an external wave model (e.g., WAM or HISWA), stored in a computer file and then input to ECOMSED. If wind wave information from an external model is unavailable, an internal wave sub-model, which is based upon shallow water SMB theory (USCOE, 1984), can be used to calculate wave parameters. The internal wave sub-model utilizes empirical formulations which provide approximate estimates of significant wave height and period; this module does not account for spatially-varying wind fields, refraction or wave breaking effects.

Once the wave parameters are specified, the Grant-Madsen wave-current model (Grant and Madsen, 1979) is used to calculate bottom shear stresses due to the interaction of waves and currents. A modified version of the Grant-Madsen model which was developed by Scott Glenn (Glenn and Grant, 1987) is incorporated into this version of ECOMSED. If the internal hydrodynamic option is used, the effect of the wave-current interaction on the bottom roughness coefficient can be calculated by the Grant-Madsen model and then included in the hydrodynamic simulation.



### 3.0 Hydrodynamic Module

#### 3.1 Introduction

This section of the user manual provides a relatively detailed description of a numerical circulation module. The module belongs to that class of models where model realism is an important goal and addresses mesoscale phenomena, that is activity characterized by 1-100 km length and tidal-30 day time scales commonly observed in estuaries and the coastal ocean [Beardsley and Boicourt, 1981]. The module is a three-dimensional coastal ocean model, incorporating a turbulence closure model to provide a realistic parameterization of the vertical mixing processes. The prognostic variables are the three components of velocity, temperature, salinity, turbulence kinetic energy, and turbulence macroscale. The momentum equations are nonlinear and incorporate a variable Coriolis parameter. Prognostic equations governing the thermodynamic quantities, temperature, and salinity account for water mass variations brought about by highly time-dependent coastal upwelling/downwelling processes as well as horizontal advective processes. Free surface elevation is also calculated prognostically, with only some sacrifice in computational time so that tides and storm surge events can also be simulated. This is accomplished by use of a mode splitting technique whereby the volume transport and vertical velocity shear are solved separately. Other computing variables include density, vertical eddy viscosity, and vertical eddy diffusivity. The module also accommodates realistic coastline geometry and bottom topography.

The hydrodynamic module, ECOM described here is a three-dimensional, time-dependent model developed by Blumberg and Mellor (1980, 1987). This module of ECOMSED, has a long history of successful applications to oceanic, coastal and estuarine waters. Some recent applications of the module include Chesapeake Bay (Blumberg and Goodrich, 1990), New York Bight (Blumberg and Galperin, 1990), Delaware Bay and Delaware River (Galperin and Mellor, 1990a, b), the Gulf Stream Region (Ezer and Mellor, 1992), Massachusetts Bay (Blumberg et al., 1993), Georges Bank (Chen et al., 1995), the Oregon Continental Shelf (Allen et al., 1995), and more recently in New York Bight and New York Harbor (Blumberg et al., 1999) and in Onondaga Lake (Ahsan and Blumburg, 1999). In all of these studies, the predictive capabilities of the module were assessed via extensive comparisons with data and a confidence has been established that the predominant physics is realistically reproduced by the module. A detailed description of the module can be found in the above referenced works.



## 3.2 The Governing Equations

## 3.2.1 Dynamic and Thermodynamic Equations

The equations which form the basis of the circulation model describe the velocity and surface elevation fields, and the temperature and salinity fields. Two simplifying approximations are used [Bryan, 1969]; first, it is assumed that the weight of the fluid identically balances the pressure (hydrostatic assumption), and second, density differences are neglected unless the differences are multiplied by gravity (Boussinesq approximation).

Consider a system of orthogonal Cartesian coordinates with x increasing eastward, y increasing northward, and z increasing vertically upwards. The free surface is located at  $z = \eta(x,y,t)$  and the bottom is at z = -H(x,y). If  $\bar{V}$  is the horizontal velocity vector with components (U,V) and  $\bar{V}$  the horizontal gradient operator, the continuity equation is:

$$\nabla \cdot \vec{\mathbf{V}} + \frac{\partial \mathbf{W}}{\partial \mathbf{Z}} = 0 \tag{3-1}$$

The Reynolds momentum equations are

$$\frac{\partial \mathbf{U}}{\partial \mathbf{t}} + \vec{\mathbf{V}} \cdot \nabla \mathbf{U} + \mathbf{W} \frac{\partial \mathbf{U}}{\partial \mathbf{z}} - \mathbf{f} \mathbf{V} = -\frac{1}{\rho_0} \frac{\partial \mathbf{P}}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{z}} \left( \mathbf{K}_{\mathrm{M}} \frac{\partial \mathbf{U}}{\partial \mathbf{z}} \right) + \mathbf{F}_{\mathrm{X}}$$
(3-2)

$$\frac{\partial V}{\partial t} + \vec{V} \cdot \nabla V + W \frac{\partial V}{\partial z} + fU = -\frac{1}{\rho_o} \frac{\partial P}{\partial y} + \frac{\partial}{\partial z} \left( K_M \frac{\partial V}{\partial z} \right) + F_Y$$
 (3-3)

$$\rho g = -\frac{\partial P}{\partial z} \tag{3-4}$$

with  $\rho_o$  the reference density,  $\rho$  the in situ density, g the gravitational acceleration, P the pressure,  $K_M$  the vertical eddy diffusivity of turbulent momentum mixing. A latitudinal variation of the Coriolis parameter, f, is introduced by use of the  $\beta$  plane approximation.

The pressure at depth z can be obtained by integrating the vertical component of the equation of motion, (3), from z to the free surface  $\eta$ , and is

$$P(x, y, z, t) = P_{atm} + g\rho_{o}\eta + g\int_{z}^{0} \rho(x, y, z', t)dz'$$
(3-5)



Henceforth, the atmospheric pressure, P<sub>atm</sub> is assumed constant.

The conservation equations for temperature and salinity may be written as

$$\frac{\partial \theta}{\partial t} + \vec{\mathbf{V}} \cdot \nabla \theta + \mathbf{W} \frac{\partial \theta}{\partial z} = \frac{\partial}{\partial z} \left[ \mathbf{K}_{H} \frac{\partial \theta}{\partial z} \right] + \mathbf{F}_{\theta}$$
 (3-6)

$$\frac{\partial S}{\partial t} + \vec{V} \cdot \nabla S + W \frac{\partial S}{\partial z} = \frac{\partial}{\partial z} \left[ K_H \frac{\partial S}{\partial z} \right] + F_s$$
 (3-7)

where  $\theta$  is the potential temperature (or in situ temperature for shallow water applications) and S is the salinity. The vertical eddy diffusivity for turbulent mixing of heat and salt is denoted as  $K_H$ . Using the temperature and salinity, the density is computed according to an equation of state of the form

$$\rho = \rho (\theta, S) \tag{3-8}$$

given by Fofonoff [1962]. The potential density is  $\rho$ , that is, the density evaluated as a function of potential temperature and salinity but at atmospheric pressure; it provides accurate density information to calculate horizontal baroclinic gradients which enter in the pressure gradient terms and the vertical stability of the water column which enters into the turbulence closure module even in deep water when pressure effects become important.

All of the motions induced by small-scale processes not directly resolved by the model grid (subgrid scale) is parameterized in terms of horizontal mixing processes. The terms  $F_x$ ,  $F_y$ ,  $F_\theta$  and  $F_S$  found in (3-2), (3-3), (3-6) and (3-7) represent these unresolved processes and in analogy to molecular diffusion can be written as

$$F_{x} = \frac{\partial}{\partial x} \left[ 2A_{M} \frac{\partial U}{\partial x} \right] + \frac{\partial}{\partial y} \left[ A_{M} \left( \frac{\partial U}{\partial y} + \frac{\partial V}{\partial x} \right) \right]$$
(3-9a)

$$F_{y} = \frac{\partial}{\partial y} \left[ 2A_{M} \frac{\partial V}{\partial y} \right] + \frac{\partial}{\partial x} \left[ A_{M} \left( \frac{\partial U}{\partial y} + \frac{\partial V}{\partial x} \right) \right]$$
(3-9b)

and

$$F_{\theta,s} = \frac{\partial}{\partial x} \left[ A_H \frac{\partial(\theta, S)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ A_H \frac{\partial(\theta, S)}{\partial y} \right]$$
(3-10)

One should note that  $F_x$  and  $F_y$  are invariant to coordinate rotation. While these horizontal diffusive terms are meant to parameterize subgrid scale processes, in practice the horizontal diffusivities,  $A_M$  and  $A_H$ , are usually required to damp small-scale computational noise. The forms for  $A_M$  and  $A_H$  are given in Sectin 8.1.2.



### 3.2.2 Turbulence Closure

The governing equations contain parameterized Reynolds stress and flux terms which account for the turbulent diffusion of momentum, heat, and salt. The parameterization of turbulence in the module described here is based on the work of Mellor and Yamada [1974].

The vertical mixing coefficients,  $K_M$  and  $K_H$ , in (3-2), (3-3), (3-6) and (3-7) are obtained by appealing to a second order turbulence closure scheme [Mellor and Yamada, 1982] which characterizes the turbulence by equations for the turbulence kinetic energy,  $q^2/2$ , and a turbulence macroscale,  $\ell$ , according to,

$$\begin{split} &\frac{\partial q^{2}}{\partial t} + \vec{\mathbf{V}} \cdot \nabla q^{2} + \mathbf{W} \frac{\partial q^{2}}{\partial z} = \frac{\partial}{\partial z} \left( \mathbf{K}_{q} \frac{\partial q^{2}}{\partial z} \right) \\ &+ 2 \mathbf{K}_{M} \left[ \left( \frac{\partial \mathbf{U}}{\partial z} \right)^{2} + \left( \frac{\partial \mathbf{V}}{\partial z} \right)^{2} \right] + \frac{2g}{\rho_{o}} \mathbf{K}_{H} \frac{\partial \rho}{\partial z} - \frac{2q^{3}}{B_{1}\ell} + \mathbf{F}_{q} \end{split} \tag{3-11}$$

and

$$\frac{\partial \left(q^{2}\ell\right)}{\partial t} + \vec{V} \cdot \nabla (q^{2}\ell) + W \frac{\partial \left(q^{2}\ell\right)}{\partial z}$$

$$= \frac{\partial}{\partial z} \left[ K_{q} \frac{\partial}{\partial z} (q^{2}\ell) \right] + \ell E_{1} K_{M} \left[ \left( \frac{\partial U}{\partial z} \right)^{2} + \left( \frac{\partial V}{\partial z} \right)^{2} \right]$$

$$+ \frac{\ell E_{1} g}{\rho_{o}} K_{H} \frac{\partial \rho}{\partial z} - \frac{q^{3}}{B_{1}} \widetilde{W} + F_{\ell}$$
(3-12)

where  $\nabla$  is the horizontal gradient operator and a wall proximity function is defined as

$$\widetilde{\mathbf{W}} = 1 + \mathbf{E}_2 \left( \frac{\ell}{\kappa \mathbf{L}} \right)^2 \tag{3-13}$$

and where

$$(L)^{-1} \equiv (\eta - z)^{-1} + (H + z)^{-1}$$
 (3-14)

Near surfaces it may be shown that both  $\ell/\kappa$  and L are equal to the distance from the surface ( $\kappa = 0.4$  is the von Karman constant) so that  $\tilde{W} = 1 + E_2$ . Far from the surfaces where  $\ell << L, \tilde{W} \simeq 1$ . The length scale provided by (3-12) is a characteristic length of the turbulent motion at any point in space or time. An alternative to (3-12)



is to use a transport equation for the dissipation rate [Hanjalic and Launder, 1972]. The former approach according to Mellor and Yamada [1982] is more consistent since it uses an equation which describes large-scale turbulence to determine the turbulent macroscale. The terms  $F_q$  and  $F_\ell$  in (3-11) and (3-12) are the horizontal mixing and are parameterized analogously to temperature and salinity by using (3-9).

While details of the closure module are rather involved, it is possible to reduce the prescription of the mixing coefficients  $K_M$ ,  $K_H$ , and  $K_q$  to the following expressions,

$$\mathbf{K}_{\mathbf{M}} \equiv \ell \mathbf{q} \mathbf{S}_{\mathbf{M}} \tag{3-15a}$$

$$\mathbf{K}_{\mathbf{H}} \equiv \ell \mathbf{q} \mathbf{S}_{\mathbf{H}} \tag{3-15b}$$

$$\mathbf{K}_{\mathbf{q}} \equiv \ell \, \mathbf{q} \, \mathbf{S}_{\mathbf{q}} \tag{3-15c}$$

The stability functions,  $S_M$ ,  $S_H$ , and  $S_q$  are analytically derived, algebraic relations functionally dependent upon  $\partial U/\partial z$ ,  $\partial V/\partial z$ ,  $g\rho_o^{-1}\partial\rho/\partial z$ , q and  $\ell$ . These relations derive from closure hypotheses described by Mellor [1973] and summarized by Mellor and Yamada [1982]. Following Galperin et al. [1988] the stability functions are:

$$S_{M} = \frac{B_{1}^{-1/3} - 3A_{1}A_{2}G_{H} \left[ \left(B_{2} - 3A_{2}\right) \left(1 - \frac{6A_{1}}{B_{1}}\right) - 3C_{1}\left(B_{2} + 6A_{1}\right) \right]}{\left[1 - 3A_{2}G_{H}\left(6A_{1} + B_{2}\right)\right] \left(1 - 9A_{1}A_{2}G_{H}\right)}$$
(3-16)

$$S_{H} = \frac{A_{2} \left( 1 - \frac{6A_{1}}{B_{2}} \right)}{1 - 3A_{2}G_{H} \left( 6A_{1} + B_{2} \right)}$$
(3-17)

$$Sq = 0.41*S_{M}$$
 (3-18)

and

$$G_{H} n = n - n \left(\frac{N\ell}{q}\right)^{2} \tag{3-19a}$$



where

$$N = \left(-\frac{g}{\rho_o} \frac{\partial \rho}{\partial y}\right)^{1/2} \tag{3-19b}$$

is the Brunt-Vaisala frequency. The empirical constants given in Mellor and Yamada (1982) are: (A1, A2, B1, B2, C1, E1, E2) = (0.92, 0.74, 16.6, 10.1, 0.08, 1.8, 1.33), respectively.

## 3.2.3 Boundary Conditions

The boundary conditions at the free surface,  $z = \eta(x,y)$ , are

$$\rho_{o} K_{M} \left( \frac{\partial U}{\partial z}, \frac{\partial V}{\partial z} \right) = \left( \tau_{ox}, \tau_{oy} \right)$$
 (3-20a)

$$\rho_o \ K_H \left( \frac{\partial \theta}{\partial z}, \frac{\partial S}{\partial z} \right) = \left( \dot{H}, \dot{S} \right) \tag{3-20b}$$

$$q^2 = B_1^{2/3} u_{\tau s}^2$$
 (3-20c)

$$q^2 \ell = 0 \tag{3-20d}$$

$$\mathbf{W} = \mathbf{U} \frac{\partial \mathbf{\eta}}{\partial \mathbf{x}} + \mathbf{V} \frac{\partial \mathbf{\eta}}{\partial \mathbf{y}} + \frac{\partial \mathbf{\eta}}{\partial \mathbf{t}}$$
 (3-20e)

where  $(\tau_{ox}, \tau_{oy})$  is the surface wind stress vector with the friction velocity,  $u_{\tau s}$ , the magnitude of the vector. It is doubtful that the mixing length goes to zero at a surface containing wind induced waves as suggested by (3-20d). The error is incurred in the near surface layers of thickness of order of the wave height. This is an area where further improvement is necessary. The quantity  $B_1^{2/3}$  is an empirical constant (6.51) arising from the turbulence closure relations. The net ocean heat flux is  $\dot{H}$  and here  $\dot{S} \equiv S(0)[\dot{E} - \dot{P}]/\rho_o$  where  $(\dot{E} - \dot{P})$  is the net evaporation-precipitation fresh water surface mass flux rate and S(0) is the surface salinity. On the side walls and bottom of the basin, the normal gradients of  $\theta$  and S are zero so that there are no advective and diffusive heat and salt fluxes across these boundaries. At the lower boundary (b),

$$\rho_{o} K_{M} \left( \frac{\partial U}{\partial z}, \frac{\partial V}{\partial z} \right) = \left( \tau_{bx}, \tau_{by} \right)$$
 (3-21a)



$$q^2 = B_1^{2/3} u_{\tau b}^2 \tag{3-21b}$$

$$q^2 \ell = 0 \tag{3-21c}$$

$$W_b = -U_b \frac{\partial H}{\partial x} - V_b \frac{\partial H}{\partial y}$$
 (3-21d)

where H(x,y) is the bottom topography and  $u_{\tau b}$  is the friction velocity associated with the bottom frictional stress  $\left(\tau_{bx},\tau_{by}\right)$ . The bottom stress is determined by matching velocities with the logarithmic law of the wall. Specifically,

$$\vec{\tau}_{h} = \rho_{o} C_{D} | \vec{V}_{h} | \vec{V}_{h}$$
(3-22)

With value of the drag coefficient C<sub>D</sub> given by

$$C_{\rm D} = \left[ \frac{1}{\kappa} \ln(H + z_{\rm b}) / z_{\rm o} \right]^{-2}$$
 (3-23a)

where  $z_b$  and  $V_b$  are the grid point and corresponding velocity in the grid point nearest the bottom and  $\kappa$  is the von Karman constant. The final result of (3-22) and (3-23) in conjunction with the turbulent closure derived  $K_M$  is that the calculations will yield

$$\vec{V} = (\vec{\tau}_b / \rho \kappa u_{\tau b}) \ln \left( \frac{H + z}{z_o} \right)$$
 (3-23b)

in the lower boundary region if enough resolution is provided. In those instances where the bottom boundary layer is not well resolved, it is more appropriate to specify  $C_D = 0.0025$ . The actual algorithm is to set  $C_D$  to the larger of the two values given by (3-23a) and 0.0025. The parameter  $z_o$  depends on the local bottom roughness; in the absence of specific information  $z_o = 1$  cm is used as suggested by Weatherly and Martin [1978].

## 3.2.4 Open Lateral Boundary Condition

## 3.2.4.1 Temperature and Salinity

Open lateral boundary conditions are problematic since one must parameterize the environment exterior to the relevant domain. Two types of open boundaries exist, inflow and outflow. Temperature and salinity are prescribed from data at an inflowing boundary, whereas at outflow boundaries,



$$\frac{\partial}{\partial t}(\theta, S) + U_n \frac{\partial}{\partial n}(\theta, S) = 0 \tag{3-23c}$$

is solved where the subscript n is the coordinate normal to the boundary. Turbulence kinetic energy and the macroscale quantity  $(q^2\ell)$  are calculated with sufficient accuracy at the boundaries by neglecting the advection in comparison with other terms in their respective equations.

The open lateral velocity boundary conditions in some of the applications are computed by using the available hydrographic data in conjunction with a simplified diagnostic model. This type of model uses only geostrophic plus Ekman dynamics and therefore solves a simplified form of the full equations of motion. It does not require a velocity at a reference level but only along a single transect crossing f/H contours. A detailed description of this module can be found in the work by Kantha et al. [1982]. While the normal component of velocity is specified, a free slip condition is used for the tangential component.

## 3.2.4.2 Water Level Boundary Condition

In developing the ocean circulation module, open boundary conditions that allow longwave energy (e.g., tides) to enter the open boundaries as well as a means of radiating out longwave energy that impacts the open boundary from the interior of the model domain must be provided. There are a number of radiation boundary conditions that can be utilized to achieve these goals. ECOMSED modeling framework adopts several types of boundary conditions that are discussed below.

## 3.2.4.2.1 Clamped Boundary Condition

In this type of boundary condition the module uses water level along the boundary grids assigned by the users either from observed data or tidal harmonics. However, this kind of boundary condition is considered rigid and does not allow long wave energy (tides or storm surges) to enter or radiate out of the model domain. For a smaller model domain where wind induced long wave is important to pass through the model boundary, the clamped boundary condition could be problematic.

### 3.2.4.2.2 Inverted Reid and Bodine Boundary Condition

For longwave to radiate through the boundaries, ECOMSED model utilizes an open boundary condition developed by Reid and Bodine (1968). This condition has the form of

$$\mathbf{\eta} = \mathbf{\eta}_{o} + \lambda_{t} \, \mathbf{u}_{n} \left[ \mathbf{g} / \mathbf{D} \right]^{-1/2} \tag{3-24a}$$

where  $\eta$  is the sea level at the open boundary,  $\eta_o$  is the known (assigned) tidal and perhaps low frequency sea level variation at the grid cell,  $u_n$  is the model-predicted velocity perpendicular to the open boundary, g is the acceleration due to gravity, and



D is the depth of the grid cell. (The LaGrange multiplier  $\lambda_t = 1$  is calculated each time step to allow modification of the sea level due to longwave radiation.) For Inverted Reid and Bodine type of boundary condition,  $\lambda_t = 1$ . Please note for  $\lambda_t = 0$  the formulation provided by Equation (3-24a) gives rise to a condition which is strictly clamped.

## 3.2.4.2.3 Optimized Clamped Boundary Condition

The optimized clamped bounary condition can be defined by Equation (3-24a). Here the LaGrange multiplier is computed with time based on solving optimization problems that minimize the difference between the model computed values and the "reference" boundary values under certain integral constraints on the open boundary. These constraints represent the energy, momentum, and mass fluxes through the open boundary. Detailed discussion on the optimized boundary conditions can be found in Shulman (1995) and Shulman and Lewis (1994).

## 3.3 Vertical Coordinate Representation

It has often been noted that the ordinary x,y,z coordinate system has certain disadvantages in the vicinity of large bathymetric irregularities. It is desirable to introduce a new set of independent variables that transforms both the surface and the bottom into coordinate surfaces [Phillips, 1957] called  $\sigma$ -coordinate system which is illustrated in Figure 3-1. The governing external and internal mode equations are transformed from (x,y,z,t) to (x\*,y\*, $\sigma$ ,t\*) coordinates, where

$$x *= x \quad y *= y \quad \sigma = \frac{z - \eta}{H + \eta}$$
  $t *= t$  (3-25)

Now let  $D \equiv H + \eta$  and apply the chain rule; the following relationships linking derivatives in the old system to those in the new system are obtained:

$$\frac{\partial G}{\partial x} = \frac{\partial G}{\partial x^*} - \frac{\partial G}{\partial \sigma} \left( \frac{\sigma}{D} \frac{\partial D}{\partial x^*} + \frac{1}{D} \frac{\partial \eta}{\partial x^*} \right)$$
(3-26a)

$$\frac{\partial G}{\partial y} = \frac{\partial G}{\partial y^*} - \frac{\partial G}{\partial \sigma} \left( \frac{\sigma}{D} \frac{\partial D}{\partial y^*} + \frac{1}{D} \frac{\partial \eta}{\partial y^*} \right)$$
(3-26b)

$$\frac{\partial G}{\partial z} = \frac{1}{D} \frac{\partial G}{\partial \sigma}$$
 (3-26c)

$$\frac{\partial G}{\partial t} = \frac{\partial G}{\partial t^*} - \frac{\partial G}{\partial \sigma} \left( \frac{\sigma}{D} \frac{\partial D}{\partial t^*} + \frac{1}{D} \frac{\partial \eta}{\partial t^*} \right)$$
(3-26d)



where G is an arbitrary field available, and  $\sigma$  ranges from  $\sigma = 0$  at  $z = \eta$  to  $\sigma = -1$  at z = -H. A new vertical velocity can now be defined

$$\omega = Wn - U\sigma \frac{\partial D}{\partial x^*} + \frac{\partial \eta}{\partial x^*} - V\sigma \frac{\partial D}{\partial y^*} + \frac{\partial \eta}{\partial y^*} - \left(\sigma \frac{\partial D}{\partial t^*} + \frac{\partial \eta}{\partial t^*}\right)$$
(3-27)

which transforms the boundary conditions, (3-20e) and (3-21d), into

$$\omega(x^*, y^*, 0, t^*) = 0 \tag{3-28a}$$

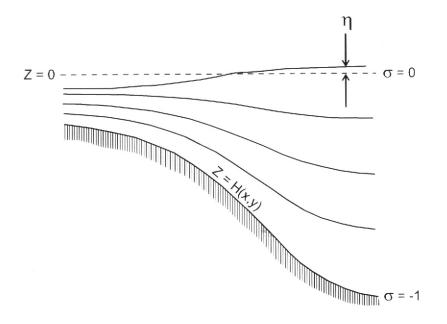
$$\omega(x^*, y^*, -1, t^*) = 0 \tag{3-28b}$$

Also, any vertically integrated quantity, G, for example, now appears as

$$\overline{\mathbf{G}} = \int_{-1}^{0} \mathbf{G} \, \mathrm{d}\boldsymbol{\sigma} \tag{3-29}$$

Equations (3-1), (3-2), (3-3), (3-6), (3-7), (3-11) and (3-12) may now be written as (all asterisks will be dropped for notational convenience)

$$\frac{\partial \eta}{\partial t} + \frac{\partial UD}{\partial x} + \frac{\partial VD}{\partial y} + \frac{\partial \omega}{\partial \sigma} = 0$$
 (3-30)





The sigma coordinate system.

FIGURE 3-1

$$\frac{\partial \text{ UD}}{\partial \text{ t}} + \frac{\partial \text{ U}^{2} \text{ D}}{\partial \text{ x}} + \frac{\partial \text{ UVD}}{\partial \text{ y}} + \frac{\partial \text{ U} \text{ \omega}}{\partial \sigma} - \text{ fVD} + \text{gD} \frac{\partial \eta}{\partial \text{ x}}$$

$$= \frac{\partial}{\partial \sigma} \left( \frac{K_{M}}{D} \frac{\partial U}{\partial \sigma} \right) - \frac{\text{gD}^{2}}{\rho_{o}} \frac{\partial}{\partial \text{x}} \int_{\sigma}^{0} \rho \, d\sigma$$

$$+ \frac{\text{gD}}{\rho_{o}} \frac{\partial D}{\partial \text{x}} \int_{\sigma}^{0} \sigma \frac{\partial \rho}{\partial \sigma} \, d\sigma + DF_{x}$$
(3-31)

$$\begin{split} &\frac{\partial \, VD}{\partial \, t} + \frac{\partial \, UVD}{\partial \, x} + \frac{\partial \, V^2 \, D}{\partial \, y} + \frac{\partial \, V \, \omega}{\partial \sigma} + f UD \, + g D \, \frac{\partial \eta}{\partial \, y} \\ &= &\frac{\partial}{\partial \sigma} \bigg( \frac{K_M}{D} \, \frac{\partial U}{\partial \sigma} \bigg) - \frac{g D^2}{\rho_o} \, \frac{\partial}{\partial y} \int_{\sigma}^0 \rho \, d\sigma \\ &+ \frac{g D}{\rho_o} \, \frac{\partial D}{\partial y} \int_{\sigma}^0 \sigma \, \frac{\partial \rho}{\partial \sigma} \, d\sigma + D F_x \end{split} \tag{3-32}$$

$$\frac{\partial \Theta D}{\partial t} + \frac{\partial \Theta UD}{\partial x} + \frac{\partial \Theta VD}{\partial y} + \frac{\partial \Theta \omega}{\partial \sigma} = \frac{\partial}{\partial \sigma} \left( \frac{K_H}{D} \frac{\partial \Theta}{\partial \sigma} \right) + D F_{\Theta}$$
(3-33)

$$\frac{\partial SD}{\partial t} + \frac{\partial SUD}{\partial x} + \frac{\partial SVD}{\partial y} + \frac{\partial S\omega}{\partial \sigma} = \frac{\partial}{\partial \sigma} \left( \frac{K_H}{D} \frac{\partial S}{\partial \sigma} \right) + DF_s$$
(3-34)

$$\frac{\partial q^{2}D}{\partial t} + \frac{\partial Uq^{2}D}{\partial x} + \frac{\partial Vq^{2}D}{\partial y} + \frac{\partial \omega q^{2}}{\partial \sigma} = \frac{\partial}{\partial \sigma} \left( \frac{K_{q}}{D} \frac{\partial q^{2}}{\partial \sigma} \right) + \frac{2K_{M}}{D} \left[ \left( \frac{\partial U}{\partial \sigma} \right)^{2} + \left( \frac{\partial V}{\partial \sigma} \right)^{2} \right] + \frac{2g}{\rho_{o}} K_{H} \frac{\partial \rho}{\partial \sigma} - \frac{2Dq^{3}}{B_{I}\ell} + DF_{q}$$
(3-35)



$$\begin{split} &\frac{2q^{2}\ell\,D}{\partial\,t} + \frac{\partial\,Uq^{2}\ell\,D}{\partial\,x} + \frac{\partial\,Vq^{2}\ell\,D}{\partial\,y} + \frac{\partial\,\omega q^{2}}{\partial\,\sigma} = \frac{\partial}{\partial\,\sigma}\,\left(\,K_{qover}\,D\,\frac{\partial\,q^{2}\ell}{\partial\,\sigma}\,\right) \\ &+ E_{I}\ell\,\left\{\,\frac{K_{M}}{D}\,\left[\,\left(\frac{\partial\,U}{\partial\,\sigma}\right)^{2} + \left(\frac{\partial\,V}{\partial\,\sigma}\right)^{2}\,\right] + \frac{q\,E^{3}}{\rho_{o}}\,K_{H}\,\frac{\partial\rho}{\partial\,\sigma}\,\right\} - \frac{Dq^{3}}{B_{I}}\,\tilde{W} + DF \end{split} \right. \end{split} \tag{3-36}$$

The horizontal viscosity and diffusion terms are defined according to:

$$F_{x} \equiv \frac{\partial D\hat{t}_{xx}}{\partial x} + \frac{\partial}{\partial y} \left( D\hat{\tau}_{yx} \right)$$
 (3-37)

$$F_{y} \equiv \frac{\partial D\hat{\tau}_{yy}}{\partial y} + \frac{\partial}{\partial x} \left( D\hat{\tau}_{xy} \right)$$
(3-38)

with

$$\hat{\tau}_{xx} = 2A_{M} \left[ \frac{\partial U}{\partial x} \right]$$
 (3-39)

$$\hat{\tau}_{xy} = \hat{\tau}_{yx} = A_M \left[ \frac{\partial U}{\partial y} + \frac{\partial V}{\partial y} \right]$$
 (3-40)

$$\hat{\tau}_{yy} = 2 A_{M} \left[ \frac{\partial V}{\partial y} \right]$$
 (3-41)

Also,

$$F_{\theta_i} \equiv \frac{\partial D \hat{q}_x}{\partial x} + \frac{\partial D \hat{q}_y}{\partial y}$$
(3-42)

$$\hat{q}_{x} = A_{H} \left[ \frac{\partial \theta_{i}}{\partial x} \right]$$
(3-43)

$$\hat{\mathbf{q}}_{y} = \mathbf{A}_{H} \left[ \frac{\partial \mathbf{\theta}_{i}}{\partial \mathbf{y}} \right]^{00} \tag{3-44}$$



where  $\theta_i$  now represents  $\theta$ , S,  $q^2$  and  $q^2\ell$ .

Mellor and Blumberg [1985] have shown that the conventional model for horizontal diffusion is incorrect when bottom topographical slopes are large. Horizontal mixing coefficient  $A_m$  and  $A_H$  for both momentum and heat/salinity are parameterized suggested by Smagorinsky (963) as described in Section 3.5.2.

## 3.4 Mode Splitting Technique

The equations governing the dynamics of coastal, estuarine and lake circulation contain propagation of fast moving external gravity waves and slow moving internal gravity waves. It is desirable in terms of computer economy to separate out vertically integrated equations (external mode) from the vertical structure equations (internal mode). This technique, known as mode splitting [see Simons, 1974; Madala and Piacsek, 1977] permits the calculation of the free surface elevation with little sacrifice in computational time by solving the volume transport separately from the vertical velocity shear.

The volume transport, external mode equations are obtained by integrating the internal mode equations over the depth, thereby eliminating all vertical structure. By integrating (3-30) from  $\sigma = -1$  to  $\sigma = 0$  and using the boundary conditions (3-28a,b) an equation for the surface elevation can be written as

$$\frac{\partial \eta}{\partial t} + \frac{\partial \overline{\mathbf{U}} \mathbf{D}}{\partial x} + \frac{\partial \overline{\mathbf{V}} \mathbf{D}}{\partial y} = 0 \tag{3-45}$$

and the momentum equations become upon vertical integration

$$\frac{\partial \overline{U}D}{\partial t} + \frac{\partial \overline{U}^{2}D}{\partial x} + \frac{\partial \overline{U}VD}{\partial y} - f\overline{V}D + gD\frac{\partial \eta}{\partial x} - D\overline{F}_{x} = -\overline{w}\overline{u}(0)$$

$$+ \overline{w}\overline{u}(-1) - \frac{\partial \overline{D}U'^{2}}{\partial x} - \frac{\partial \overline{D}U'V'}{\partial y} - \frac{gD^{2}}{\rho_{o}}\frac{\partial}{\partial x}\int_{-1}^{\circ}\int_{\sigma}^{\circ}\rho d\sigma'd\sigma$$

$$+ \frac{gD}{\rho_{o}}\frac{\partial D}{\partial x}\int_{-1}^{\circ}\int_{\sigma}^{\circ}\sigma'\frac{\partial \rho}{\partial \sigma} d\sigma'd\sigma$$
(3-46)



$$\begin{split} \frac{\partial \overline{V}D}{\partial t} + \frac{\partial \overline{U}VD}{\partial x} + \frac{\partial \overline{V}^{2}D}{\partial y} + f\overline{U}D + gD\frac{\partial \eta}{\partial y} - D\overline{F}_{y} &= -\overline{wv}(0) \\ + \overline{wv}(-1) - \frac{\partial D\overline{U'V'}}{\partial x} - \frac{\partial \overline{DV'^{2}}}{\partial y} - \frac{gD^{2}}{\rho_{o}} \frac{\partial}{\partial y} \int_{-1}^{\circ} \int_{\sigma}^{\circ} \rho \, d\sigma' d\sigma \\ + \frac{gD}{\rho_{o}} \frac{\partial D}{\partial y} \int_{-1}^{\circ} \int_{\sigma}^{\circ} \sigma' \frac{\partial \rho}{\partial \sigma'} d\sigma' d\sigma \end{split} \tag{3-47}$$

where the pressure has been obtained from (3-5) and the vertically integrated velocities are defined as

$$(\overline{\mathbf{U}}, \overline{\mathbf{V}}) \equiv \int_{-1}^{0} (\mathbf{U}, \mathbf{V}) d\sigma$$
 (3-48)

The wind stress components are  $-\overline{wu}(0)$ , and  $-\overline{wv}(0)$ , and the bottom stress components are  $-\overline{wu}(-1)$  and  $-\overline{wv}(-1)$ . The terms in (3-46) and (3-47) involving U'<sup>2</sup>, U'V', and V'<sup>2</sup> represent vertical averages of the cross-products of the velocity departures from the vertically integrated (average) velocity and are often denoted as the dispersion terms. Thus

$$\left(\overline{\mathbf{U}^{\prime 2}}, \overline{\mathbf{V}^{\prime 2}}, \overline{\mathbf{U}^{\prime} \mathbf{V}^{\prime}}\right) = \int_{-1}^{0} \left(\mathbf{U}^{\prime 2}, \mathbf{V}^{\prime 2}, \mathbf{U}^{\prime} \mathbf{V}^{\prime}\right) d\sigma \tag{3-49}$$

where  $(U',V')=(U-\overline{U},V-\overline{V})$ . The quantities  $\overline{F}_x$  and  $\overline{F}_y$  are vertical integrals of the horizontal momentum diffusion and are defined according to

$$\overline{DF}_{x} = \frac{\partial}{\partial x} \left( 2A_{M} \frac{\partial \overline{U}D}{\partial x} \right) + \frac{\partial}{\partial y} A_{M} \left( \frac{\partial \overline{U}D}{\partial y} + \frac{\partial \overline{V}D}{\partial x} \right)$$
(3-50)

$$D\overline{F}_{y} = \frac{\partial}{\partial y} \left( 2A_{M} \frac{\partial \overline{V}D}{\partial y} \right) + \frac{\partial}{\partial x} A_{M} \left( \frac{\partial \overline{U}D}{\partial y} + \frac{\partial \overline{V}D}{\partial x} \right)$$
(3-51)

The computational strategy is to solve equations for the external mode, the shallow water wave equations (3-45), (3-46), and (3-47), with a short time step to resolve tidal motions. The external mode solutions are obtained with the terms on the right-hand side of (3-46) and (3-47) held fixed in time and after a large number of time steps, of the order of 100, an internal mode calculation is carried out. The external mode provides  $\partial \eta/\partial x$  and  $\partial \eta/\partial y$  for insertion into the internal mode equations, (3-30) through (3-36), which are then solved with a much longer time step. Once the vertical



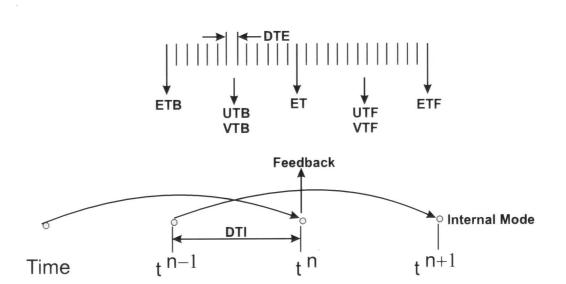
structure has been determined, the terms on the right-hand side (3-46) and (3-47) are updated and another external mode solution begins. In future simulations, the advective and diffusive terms in (3-46) and (3-47) will be supplied by the internal mode. Figure 3-2 illustrates the time stepping process for the external and internal mode.

The external mode equations have not been subtracted from the original equations (3-30) and (3-32) to form the more conventional internal mode set as, for example, in Bryan [1969] and Wang [1982]. Consequently there may be a slow tendency for the vertical integral of the internal mode velocities to differ from the external mode velocities. This arises because of different truncation errors in each mode. To insure against accumulated mismatch, the vertical mean of the internal velocity is replaced at every time step by the external mode velocity.

## 3.5 Orthogonal Curvilinear Coordinate System Transformation

An important advantage of the present model over that used earlier is the use of a horizontal, orthogonal, curvilinear coordinate system. The full set of the equations in given in Blumberg and Herring (1987); for the present version of the primer only the internal mode equations are given. These equations in the mass flux conservative form are:







A simplified illustration of the interaction of the External Mode and the Internal Mode

The Continuity Equation

$$\mathbf{h}_{1}\mathbf{h}_{2} \frac{\partial \mathbf{\eta}}{\partial \mathbf{t}} + \frac{\partial}{\partial \boldsymbol{\xi}_{1}} \left(\mathbf{h}_{2}\mathbf{U}_{1}\mathbf{D}\right) + \frac{\partial}{\partial \boldsymbol{\xi}_{2}} \left(\mathbf{h}_{1}\mathbf{U}_{2}\mathbf{D}\right) + \mathbf{h}_{1}\mathbf{h}_{2} \frac{\partial \boldsymbol{\omega}}{\partial \boldsymbol{\sigma}} = \mathbf{0}$$
 (3-52a)

where:

$$\omega = W - \frac{1}{h_1 h_2} \left[ h_2 U_1 \left( \sigma \frac{\partial D}{\partial \xi_1} + \frac{\partial \eta}{\partial \xi_1} \right) + h_1 U_2 \left( \sigma \frac{\partial D}{\partial \xi_2} + \frac{\partial \eta}{\partial \xi_2} \right) \right]$$

$$- \left( \sigma \frac{\partial D}{\partial t} + \frac{\partial \eta}{\partial t} \right)$$
(3-52b)

<u>Free Surface Equation</u>
The Reynolds Equations

$$\begin{split} &\frac{\partial (h_1 h_2 D U_1)}{\partial t} + \frac{\partial}{\partial \xi_1} (h_2 D U_1^2) + \frac{\partial}{\partial \xi_2} (h_1 D U_1 U_2) + h_1 h_2 \frac{\partial (\omega U_1)}{\partial \sigma} \\ &+ D U_2 \left( - U_2 \frac{\partial h_2}{\partial \xi_1} + U_1 \frac{\partial h_1}{\partial \xi_2} - h_1 h_2 f \right) \\ &= - g D h_2 \left( \frac{\partial \eta}{\partial \xi_1} + \frac{\partial H_o}{\partial \xi_1} \right) - \frac{g D^2 h_2}{\rho_o} \int_{\sigma}^{o} \left[ \frac{\partial \rho}{\partial \xi_1} - \frac{\sigma}{D} \frac{\partial D}{\partial \xi_1} \frac{\partial \rho}{\partial \sigma} \right] d\sigma \end{split}$$

$$\begin{split} & - D \frac{h_2}{\rho_o} \; \frac{\partial P_a}{\partial \xi_1} \; + \frac{\partial}{\partial \xi_1} \left( 2 A_M \; \frac{h_2}{h_1} \; D \; \frac{\partial U_1}{\partial \xi_1} \right) \; + \; \frac{\partial}{\partial \xi_2} \left( A_M \; \frac{h_1}{h_2} \; D \; \frac{\partial U_1}{\partial \xi_2} \right) \\ & + \; \frac{\partial}{\partial \xi_2} \left( A_M \; D \; \frac{\partial U_2}{\partial \xi_1} \right) \; + \; \frac{h_1 h_2}{D} \; \frac{\partial}{\partial \sigma} \left( K_M \; \frac{\partial U_1}{\partial \sigma} \right) \end{split}$$

(3-53)



$$\frac{\partial (\mathbf{h}_{1}\mathbf{h}_{2}\mathrm{D}\mathbf{U}_{2})}{\partial \mathbf{t}} + \frac{\partial}{\partial \xi_{1}} (\mathbf{h}_{2}\mathrm{D}\mathbf{U}_{1}\mathbf{U}_{2}) + \frac{\partial}{\partial \xi_{2}} (\mathbf{h}_{1}\mathrm{D}\mathbf{U}_{2}^{2}) + \mathbf{h}_{1}\mathbf{h}_{2}\frac{\partial (\mathbf{\omega}\mathbf{U}_{2})}{\partial \sigma}$$

$$+ \mathrm{D}\mathbf{U}_{1} \left( - \mathbf{U}_{1} \frac{\partial \mathbf{h}_{1}}{\partial \xi_{2}} + \mathbf{U}_{2} \frac{\partial \mathbf{h}_{2}}{\partial \xi_{1}} + \mathbf{h}_{1}\mathbf{h}_{2} \mathbf{f} \right)$$

$$= - \mathrm{gDh}_{1} \left( \frac{\partial \eta}{\partial \xi_{2}} + \frac{\partial \mathbf{H}_{0}}{\partial \xi_{2}} \right) - \frac{\mathrm{gD}^{2}\mathbf{h}_{1}}{\rho_{0}} \int_{\sigma}^{\sigma} \left[ \frac{\partial \rho}{\partial \xi_{2}} - \frac{\sigma}{\mathrm{D}} \frac{\partial D}{\partial \xi_{2}} \frac{\partial \rho}{\partial \sigma} \right] d\sigma$$

$$- \mathrm{D}\frac{\mathbf{h}_{1}}{\rho} \frac{\partial \mathrm{P}_{a}}{\partial \xi_{2}} + \frac{\partial}{\partial \xi_{2}} \left( 2\mathbf{A}_{M} \frac{\mathbf{h}_{1}}{\mathbf{h}_{2}} \mathrm{D} \frac{\partial \mathbf{U}_{2}}{\partial \xi_{2}} \right) + \frac{\partial}{\partial \xi_{1}} \left( \mathbf{A}_{M} \frac{\mathbf{h}_{2}}{\mathbf{h}_{1}} \mathrm{D} \frac{\partial \mathbf{U}_{2}}{\partial \xi_{1}} \right)$$

(3-54)

Transport of Temperature

$$\begin{split} & h_1 h_2 \; \frac{\partial (\theta \, D)}{\partial t} \; + \; \frac{\partial}{\partial \xi_1} (h_2 U_1 \theta \, D) \; + \; \frac{\partial}{\partial \xi_2} (h_1 U_2 \theta \, D) \; + \; h_1 h_2 \; \frac{\partial (\omega \, \theta)}{\partial \sigma} \\ \\ & = \; \frac{\partial}{\partial \xi_1} \; \left( \frac{h_2}{h_1} \; A_H D \; \frac{\partial \theta}{\partial \xi_1} \right) \; + \; \frac{\partial}{\partial \xi_2} \left( \frac{h_1}{h_2} \; A_H D \; \frac{\partial \theta}{\partial \xi_2} \right) \; + \; \frac{h_1 h_2}{D} \; \frac{\partial}{\partial \sigma} \; \left( K_H \; \frac{\partial \theta}{\partial \sigma} \right) \end{split}$$

 $+ \frac{\partial}{\partial \xi} \left( A_{M} D \frac{\partial U_{1}}{\partial \xi} \right) + \frac{h_{1}h_{2}}{D} \frac{\partial}{\partial \sigma} \left( K_{M} \frac{\partial U_{2}}{\partial \sigma} \right)$ 

(3-55)



Transport of Salinity

$$h_{1}h_{2} \frac{\partial(SD)}{\partial t} + \frac{\partial}{\partial \xi_{1}} (h_{2}U_{1}SD) + \frac{\partial}{\partial \xi_{2}} (h_{1}h_{2}SD) + h_{1}h_{2} \frac{\partial(\omega S)}{\partial \sigma}$$

$$= \frac{\partial}{\partial \xi_{1}} \left( \frac{h_{2}}{h_{1}} A_{H}D \frac{\partial S}{\partial \xi_{1}} \right) + \frac{\partial}{\partial \xi_{2}} \left( \frac{h_{1}}{h_{2}} A_{H}D \frac{\partial S}{\partial \xi_{2}} \right) + \frac{h_{1}h_{2}}{D} \frac{\partial}{\partial \sigma} \left( K_{H} \frac{\partial S}{\partial \sigma} \right)$$
(3-56)

Transport of Turbulent Kinetic Energy

$$\begin{split} & h_1 h_2 \; \frac{\partial (q^2 D)}{\partial t} \; + \; \frac{\partial}{\partial \xi_1} \; \left( h_2 U_1 D q^2 \right) \; + \; \frac{\partial}{\partial \xi_2} \; \left( h_1 U_2 D q^2 \right) \; h_1 h_2 \frac{\partial (\omega q^2)}{\partial \sigma} \\ & = \; h_1 h_2 \! \left[ \! \frac{\left( \partial U_1 \right)^2}{D} \left( \left( \frac{\partial U_1}{\partial \sigma} \right)^2 \; + \; \left( \frac{\partial U_2}{\partial \sigma} \right)^2 \right] \; + \; \frac{2g}{\rho_o} \; K_H \; \frac{\partial \rho}{\partial \sigma} \; - \; \frac{2q^3 D}{\Lambda_1} \right\} \\ & + \; \frac{\partial}{\partial \xi_1} \; \left( \frac{h_2}{h_1} \; A_H D \; \frac{\partial q^2}{\partial \xi_1} \right) \; + \; \frac{\partial}{\partial \xi_2} \! \left( \frac{h_1}{h_2} \; A_H D \; \frac{\partial q^2}{\partial \xi_2} \right) \; + \; \frac{h_1 h_2}{D} \; \frac{\partial}{\partial \sigma} \; \left( K_q \; \frac{\partial q^2}{\partial \sigma} \right) \end{split}$$

(3-57)

Turbulent Macroscale

$$\begin{split} & h_1 h_2 \; \frac{\partial (q^2 \lambda D)}{\partial t} \; + \; \frac{\partial}{\partial \xi_1} \; (h_2 U_1 D q^2 \lambda) \; + \; \frac{\partial}{\partial \xi_2} \; (h_1 U_2 D q^2 \lambda) \; + \; h_1 h_2 \; \frac{\partial (\omega q^2 \lambda)}{\partial \sigma} \\ & = \; h_1 h_2 \; \bigg\{ \frac{\lambda E_1 K_M}{D} \; \bigg[ \bigg( \frac{\partial U_1}{\partial \sigma} \bigg)^2 \; + \; \bigg( \frac{\partial U_2}{\partial \sigma} \bigg)^2 \bigg] \; + \; \frac{\lambda E_1 g}{\rho_o} \; K_H \; \frac{\partial \rho}{\partial \sigma} \; - \; \frac{q^3 D}{B_1} \; \tilde{w} \bigg\} \\ & \quad + \; \frac{\partial}{\partial \xi_1} \; \bigg( \frac{h_2}{h_1} \; A_H D \; \frac{\partial (q^2 \lambda)}{\partial \xi_1} \bigg) \; + \; \frac{\partial}{\partial \xi_2} \bigg( \frac{h_1}{h_2} \; A_H D \; \frac{\partial (q^2 \lambda)}{\partial \xi_2} \bigg) \end{split}$$



$$+ \frac{\mathbf{h}_1 \mathbf{h}_2}{\mathbf{D}} \frac{\partial}{\partial \mathbf{\sigma}} \left( \mathbf{K}_q \frac{\partial (\mathbf{q}^2 \boldsymbol{\lambda})}{\partial \mathbf{\sigma}} \right) \tag{3-58}$$

where  $\xi_1$  and  $\xi_2$  are arbitrary horizontal curvilinear orthogonal coordinates.

### 3.6 Surface Heat Flux

The energy content in lakes, reservoirs, estuaries, and coastal and oceanic water bodies is primarily governed by the surface heat energy exchanges. Measurements of heat fluxes such as solar radiations, atmospheric radiation, sensible heat and latent heat fluxes are very difficult and costly to make and are often parameterized to obtain the fluxes, using the most commonly available meteorological data. The processes that control the heat exchange between the water and atmosphere are well documented (Large and Pond, 1982; Rosati and Miyakoda, 1988; Cole and Buchak, 1994; Ahsan and Blumberg, 1999). All of these works relied mostly on the bulk formulae to evaluate the components of the heat budget. It is important to note here that most of bulk formulae, available in literature, for calculations of radiative fluxes are based on basically the same principles and generally agree with one another in general patterns of temporal and spatial variations of fluxes. However, significant differences in their magnitudes exist depending on the time period of the year and latitudinal position of the study area.

Estimation of net heat flux requires a great deal of judgement in choosing the bulk formulae which are dependent on meteorological parameters like cloud cover, relative humidity, air temperature, winds, water surface temperature etc. Computations of four major heat flux components such as short wave solar radiations, longwave atmospheric radiations, sensible heat and latent heat fluxes have been introduced in ECOM code using three formulations based on the works of Ahsan and Blumberg (1999), Rosati and Miyakoda (1988) and Large and Pond (1982). Users may choose either of these three formulations by choosing heat flux options A&BFLX, R&BFLX, and L&PFLX respectively (see data entry section). Table 3-1 describes the equations to compute the individual heat flux component using these three options. It has been demonstrated in literature that option A&BFLX has more success in simulating heat budget in inland lakes, reservoirs and estuarine systems. The latter two options are described as more appropriate for oceanic environments. The users may apply their judgement to choose these options depending on the nature of their applications.



Table 3-1.	Heatflux Formulations in Ecom Model					
	A and BFLX	R and MFLX	L and PFLX			
Solar Radiation* (H <sub>s</sub> )	users measured data	users measured data	users measured data			
Atmospheric Radiation (H <sub>a</sub> )	$\varepsilon\sigma \left\{ \frac{\left(9.37x10^{-6}T_{a}^{6}\right)}{\left(1+0.17C^{2}\right)-T_{s}^{4}}\right\} \varepsilon$	$c\sigma T_{a}^{4} \left(0.39 - 0.05e_{a}^{1/2}\right)$ 1-0.8C)+4 $\epsilon\sigma T_{s}^{3} \left(T_{s} - T_{a}\right)$	$\begin{cases} \epsilon \sigma T_{s}^{4} \left(0.39 - 0.05 e_{s}^{1/2}\right) \\ +4\epsilon \sigma T_{s}^{3} \left(T_{s} - T_{a}\right) \end{cases}$ $\left(1 - 0.62C^{2}\right)$			
Sensible Heatflux (H <sub>c</sub> )	$C_c f(w)(T_s - T_a)$	$C_TW(T_s-T_a)$	$C_T U_z (T_s - \theta_z)$			
Evaporative Heatflux (H <sub>e</sub> )	$f(w)(e_s - e_a)$	$C_{\rm E}W(e_{\rm s}-re_{\rm a})0.621/P$	$C_E U_x (\theta_s - \theta_x)$			
References	Ahsan & Blumberg (1999) (Cole & Buchak (1994))	Rosati & Miyakoda (1988)	Large & Pond (1982)			

\*In case field measurements are not available, the model computes solar radiation based on:

$$\begin{split} &H_s = Q_{TOT}(1\text{-}0.62C + 0.001\partial\beta)(1\text{-}\alpha) \; ; \; Q_{TOT} = Q_{DIR} + Q_{DIFF} \; ; \; Q_{DIR} = Q_o \text{T}^{secz} \; ; \\ &Q_{DIFF} = [(1\text{-}A_a)Q_o \text{-}Q_{DIR}]/2 \; ; \; Q_o = \frac{J_o}{a^2} \; \text{CsozD}_F(\varphi,\lambda) \end{split}$$

(See Rosati and Miyakoda (1988) for definition of parameters.)

Definition of Parameters					
	€	Emmissivity of water (0.97)	CT	Bulk transfer coefficient for conductive	
	σ	Stephen-Boltzman Constant		heat flux	
		(5.67 * 10 <sup>-8</sup> ) (WM <sup>-2</sup> K <sup>-4</sup> )	CE	Bulk transfer coefficient for evaporative	
	T <sub>s</sub>	Water surface temperature in		heat flux	
		<sup>o</sup> K	W	Windspeed in m/s	
	$T_{a}$	Air temperature in <sup>o</sup> K	θ	Virtual air temperature	
	e <sub>s</sub> (Ta,Ts)		f(w)	Windspeed function (6.9 + 0.34 W <sup>2</sup> ) in w	
		mbar at air temperature T <sub>a</sub>		m <sup>-2</sup> mbar <sup>-1</sup>	
		and sea surface temperature	Р	Barometric pressure in mbar	
		$T_s$	R	relative humidity	
	С	Cloud cover fraction (0 - 1.0)			



# 4.0 Tracer/Pathogen Fate Module

Abundances of enteric organisms in natural systems are determined by rates of inputs (loads) to the bay from outfalls and shoreline sources, transport due to currents, and dispersion and loss processes that include phototoxicity, temperature, salinity, predation or die-off and settling. These factors may be present in varying degrees depending on the specific situation and locations. The resultant distribution of the organism concentration will then reflect the decay (or growth) of the organism as a function of spatial and temporal scales of the water body. The governing equation is the classical time-dependent three-dimensional mass transport equation with sink terms representing the various loss processes as described below:

$$\frac{\partial C}{\partial t} + \frac{\partial C u}{\partial x} + \frac{\partial C v}{\partial y} + \frac{\partial C w}{\partial z} = \frac{\partial}{\partial z} \left( K_H \frac{\partial C}{\partial z} \right) + F_c + kC$$

Where, C is the concentration of pathogen organism, k is the die-off coefficient or decay rate, Fc represents the horizontal diffusion of pathogen bacteria. All other terms as same as described earlier.

Populations of coliforms exhibit a number of mortality patterns in laboratory experiments when wastewater is diluted by water in an effort to simulate the discharge of a waste into a receiving water (Mancini, 1978). These patterns can be classified as first order mortality of coliforms, initial population increases followed by first order mortality and either of the above patterns, followed by a reduced rate of mortality as time increases and population levels are reduced. Initial estimates of the die-off coefficient were developed from special laboratory studies and from values reported in the literature (Mancini, 1978). Laboratory studies indicated that the coliforms bacteria die-off rate (at 20°C) in seawater varied between 0.8/day and 1.4/day. These rates are approximately equal to die-off rates developed in other modeling calibration analyses. These laboratory values confirmed the following functional relationship of the coliforms bacteria die-off rate:

$$k=k_d+k_i+k_s$$

k<sub>d</sub> = rate coefficient for death in the dark; includes effects of temperature, salinity and predation (d<sup>-1</sup>).

 $k_i$  = rate coefficient for death as mediates by irradiance ( $d^{-1}$ ).

 $k_s$  = rate coefficient for sedimentation loss ( $d^{-1}$ ).

k<sub>d</sub> is defined by Maveim (1978) and also reported by Thomann and Mueller (1987).

$$k_{d}$$
 = (0.80 + 0.006 \* (% of seawater)) x  $\pmb{\theta}^{\text{T-20}}$ 

here  $\theta = 1.07$  is dimensionless constant which describes the relationship between the rate coefficient and temperature



% of seawater for 22 ppt, for example is 22/35 x 100 (sea water 35 ppt) = 62.85%

$$k_i = \frac{\alpha I_o}{k_e z} \left[ 1 - e^{-k_e z} \right]$$

 $k_i$  = coliform mortality rate due to light ( $d^{-1}$ )

 $\alpha$  = proportionality constant

I<sub>o</sub> = average daily solar (surface) radiation (langleys/hr)

Note:

 $1 \text{ watt/m}^2 = 2.066115 \text{ langley/day}$ = 0.086088 langleys/hr.

= light extinction coefficient (m<sup>-1</sup>)

= depth of water at which the decay rate is applied

α

$$k_s = \frac{v_s}{H} = \frac{v_s}{z}$$

= net loss rate in m/day of the particulate bacterial forms.

z, H = water depth at which the rate is applied.

 $\boldsymbol{v}_{s}$  varies from 1 · 17 to 2 · 4 m/day for small (0.45-10  $\mu m)$  and large (>10 μm), grain sizes, respectively.



# 5.0 Particle Tracking Module

The movement of particles can be determined by exploiting the equivalency between tracking particles and solving a mass transport equation for a conservative substance (Thompson and Gelhar 1990). Following Dimou and Adams (1993), a random-walk particle tracking scheme has been designed which calculates the displacement of particles as the sum of an advective deterministic component and an independent, random Markovian component which statistically approximates the dispersion characteristics of the environment. By relating the advective and Markovian components to the appropriate terms in a conservation equation, a technique has been designed where a distribution of particles will turn out to be the same as that concentration resulting from the solution of the conservation equation.

In a three dimensional environment, a conservative substance is transported under the influence of advection and dispersion processes. The solution for this transport problem is commonly based on the mass balance equation. Introducing the *s* transformation in the vertical:

$$\sigma = \frac{z - \eta}{H + \eta} \tag{5-1}$$

where H(x,y) is the water depth,  $\eta(x,y)$  is the surface elevation and D = H +  $\eta$ , the transport equation for a conservative tracer in an orthogonal curvilinear coordinate system ( $\xi_1, \xi_2, \sigma$ ) can be written as (Zhang, 1995),

$$\begin{split} & h_{1}h_{2}\frac{\partial(DC)}{\partial t} + \frac{\partial}{\partial\xi_{1}}\left(h_{2}U_{1}DC\right) + \frac{\partial}{\partial\xi_{2}}(h_{1}U_{2}DC) + h_{1}h_{2}\frac{\partial(\omega C)}{\partial\sigma} \\ & = \frac{\partial}{\partial\xi_{1}}\left(\frac{h_{2}}{h_{1}}A_{H}D\frac{\partial C}{\partial\xi_{1}}\right) + \frac{\partial}{\partial\xi_{2}}\left(\frac{h_{1}}{h_{2}}A_{H}D\frac{\partial C}{\partial\xi_{2}}\right) + \frac{h_{1}h_{2}}{D}\frac{\partial}{\partial\sigma}\left(K_{H}\frac{\partial C}{\partial\sigma}\right) \end{split} \tag{5-2}$$

where

$$\omega = W - \frac{1}{h_1 h_2} \left[ h_2 U_1 \left( \sigma \frac{\partial D}{\partial \xi_1} + \frac{\partial \eta}{\partial \xi_1} \right) + h_1 U_2 \left( \sigma \frac{\partial D}{\partial \xi_2} + \frac{\partial \eta}{\partial \xi_2} \right) \right] - \left( \sigma \frac{\partial D}{\partial t} + \frac{\partial \eta}{\partial t} \right)$$
(5-3)

C is the concentration,  $h_1$  and  $h_2$  are the metrics of the unit grid cell in the  $\xi_1$  and  $\xi_2$  directions, and U1 and U2 are the velocity components along the  $\xi_1$  and  $\xi_2$  directions. Adding:



$$\frac{\partial}{\partial \xi_{1}} \left[ \frac{\partial}{\partial \xi_{1}} \left( \frac{A_{H}}{h_{1}^{2}} h_{1} h_{2} D \right) C \right] + \frac{\partial}{\partial \xi_{2}} \left[ \frac{\partial}{\partial \xi_{2}} \left( \frac{A_{H}}{h_{2}^{2}} h_{1} h_{2} D \right) C \right] + \frac{\partial}{\partial \sigma} \left[ \frac{\partial}{\partial \sigma} \left( \frac{K_{H}}{D^{2}} h_{1} h_{2} D \right) C \right]$$
(5-4)

on both sides of Equation (5-2) and rearranging it, the transport equation becomes,

$$\begin{split} &\frac{\partial}{\partial t} \left( h_1 h_2 DC \right) + \frac{\partial}{\partial \xi_1} \left\{ \left[ \frac{U_1}{h_1} + \frac{1}{h_1 h_2 D} \frac{\partial}{\partial \xi_1} \left( \frac{A_H}{h_2^2} h_1 h_2 D \right) \right] h_1 h_2 DC \right\} \\ &+ \frac{\partial}{\partial \xi_2} \left\{ \left[ \frac{U_2}{h_2} + \frac{1}{h_1 h_2 D} \frac{\partial}{\partial \xi_2} \left( \frac{A_H}{h_2^2} h_1 h_2 D \right) \right] h_1 h_2 DC \right\} \\ &+ \frac{\partial}{\partial \sigma} \left\{ \left[ \frac{\omega}{D} + \frac{1}{h_1 h_2 D} \frac{\partial}{\partial \sigma} \left( \frac{K_H}{D_2} h_1 h_2 D \right) \right] h_1 h_2 DC \right\} \\ &= \frac{\partial}{\partial \xi_1^2} \left( \frac{A_H}{h_1^2} h_1 h_2 DC \right) + \frac{\partial}{\partial \xi_2^2} \left( \frac{A_H}{h_1^2} h_1 h_2 DC \right) + \frac{\partial^2}{\partial \sigma^2} \left( \frac{K_H}{D^2} h_1 h_2 DC \right) \end{split}$$
(5-5)

Representing the conservative tracer concentration by a collection of particles, the transport problem can also be solved by particle tracking models (Dimou, 1989; Dimou and Admas 1993; Tompson and Gelhar, 1990). As described by those previous studies, the displacement of a particle in a random-walk model is governed by the non-linear Langevin equation (Gardinar, 1985)

$$\frac{\vec{dX}}{dt} = A(\vec{X}t) + B(\vec{X},t) Z_n$$
 (5-6)

where  $\vec{X}(t)$ ,  $A(\vec{X},t)$  and  $B(\vec{X}t)$  are vectors,  $\vec{X}(t)$  defines the position of a particle,  $A(\vec{X},t)$  is the deterministic forces that advect particles,  $B(\vec{X},t)$  represents the random forces that lead to particle diffusion (Solomon et al 1994), and Z(t) is a vector of the independent random numbers with zero mean and unit variance.

If  $f = f(\vec{X}, t | \vec{X}_0 t_0)$  is defined as the conditional probability density function for

X(t) of particles whose initial position at  $t_0$  is  $X_0$ , the number density will satisfy the Ito-Fokker-Planck equation (Kinzelbach, 1988; Tompson and Gelhar, 1990) in the limit as the number of particles gets very large and the time step used to solve the conservation equation gets very small.



$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial \vec{X}} (Af) = \nabla^2 \left( \frac{1}{2} BB^T f \right)$$
 (5-7)

Therefore, the transport equation (5-5) is equivalent to the Ito-Fokker-Planck equation (5-7) if  $f = h_1 h_2 DC$ ,

$$A \equiv \begin{bmatrix} \frac{U_1}{h_1} + \frac{1}{h_1 h_2 D} \frac{\partial}{\partial \xi_1} \left( \frac{A_H}{h_1^2} h_1 h_2 D \right) \\ \frac{U_2}{h_2} + \frac{1}{h_1 h_2 D} \frac{\partial}{\partial \xi_2} \left( \frac{A_H}{h_2^2} h_1 h_2 D \right) \\ \frac{\omega}{D} + \frac{1}{h_1 h_2 D} \frac{\partial}{\partial \sigma} \left( \frac{K_H}{D^2} h_1 h_2 D \right) \end{bmatrix}$$
(5-8)

and

$$\frac{1}{2}BB^{T} \equiv \begin{bmatrix} \frac{A_{H}}{h_{1}^{2}} & 0 & 0 \\ 0 & \frac{A_{H}}{h_{2}^{2}} & 0 \\ 0 & 0 & \frac{K_{H}}{D^{2}} \end{bmatrix}$$
(5-9)

Thus,  $A(\vec{X},t)$ ,  $B(\vec{X},t)$  in Equation (5-6) can be determined and the position  $\vec{X}(t)$  of each particle can be calculated.

The numerical algorithm used in the solution of Equation (5-6) is based on the same grid structure and interpolation schemes that are built into ECOMSED. To ensure that the tracking methodology is correct, tests comparing the methodology with analytical solutions were conducted (Zhang 1995). The tests involve long straight channels, with flat and sloping bottoms and circular channels with open and closed lateral boundaries. The methodology was able to obtain the correct answer for all of these test cases.



# 6.0 Sediment Transport Module

### 6.1 Introduction

The SED module is HydroQual's state-of-the-art three-dimensional sediment transport model. It realistically simulates cohesive and noncohesive sediments in a variety of aquatic systems (e.g., lakes, rivers, estuaries, bays and coastal waters). There are two different sediment transport modeling frameworks incorporated in ECOMSED. In the mid 1990s, concepts of cohesive sediment resuspension, settling and consolidation (Lick et al., 1994) were incorporated within the ECOM modeling framework to create ECOMSED (SEDZL). Over a period of several years, significant modifications were made to ECOMSED to include generalized open boundary conditions, tracers, better bottom shear stresses through a submodel for bottom boundary layer physics, surface wind-wave models, noncohesive sediment transport, and dissolved and sediment-bound tracer capabilities. ECOMSED have been used in a number of sediment transport studies, including: Pawtuxet River in Rhode Island (Ziegler and Nisbet, 1994), Watts Bar Reservoir in Tennessee (Ziegler and Nisbet, 1995), Lavaca Bay in Texas (HydroQual, 1998), Tannery Bay in Michigan (Cannelton Industries, 1998), and Green Bay in Wisconsin (Shrestha et al., 2000). In 2007, peer-reviewed sediment transport model (SEDZLJ) (Jones and Lick, 2001) was incorporated into HydroQual's hydrodynamic model framework, ECOMSED. SEDZLJ uses measured gross erosion rates from a Sedflume study (McNeil et al., 1996; Jepsen et al., 1997; Roberts et al., 1998) performed at the water body to be modeled to determine the resuspension rates of fine-grained sediment beds and measured erosion rates for sand sized sediments obtained from the literature (Roberts et al., 1998) for noncohesive sediment beds as the basis to compute sediment transport. The incorporation of SEDZLJ into ECOMSED was performed by Dr. Craig Jones (developer of the SEDZLI computer code) of Sea Engineering, Inc. (SEI). The resulting computer code was peer-reviewed by Dr. Earl Hayter of the USEPA and was applied for the cap erosion analysis of the Lower Passaic River (HydroQual, 2007).

The SED module is configured to run in conjunction with the hydrodynamic model and a wave model (if waves are included). SED uses the same numerical grid, structure and computational framework as the hydrodynamic model. Sediment dynamics inherent in the model includes sediment resuspension, transport and deposition of cohesive and noncohesive sediments. SEDZL modeling framework is discussed in Section 6.2 and SEDZLJ modeling framework is presented in Section 6.3.

### 6.2 SEDZL Modeling Framework

Cohesive sediments, as referred to herein, represent fine-grained sediments and tailings of particle diameters less than 75  $\mu$ m (clay-silt range), while noncohesive sediments are coarser particles with diameters between 75 - 500  $\mu$ m (fine-medium sand range). Coarse sand and gravel, with particle diameters greater than 500  $\mu$ m, are moved as bed load transport, which is not considered in this model because coarse-grained sediments normally comprise a small fraction of the bed in estuarine and ocean systems. Neglecting bed load will thus have negligible effect on the model results.



Both resuspension and deposition mechanisms depend upon the shear stress induced at the sediment-water interface. Computation of bottom shear stresses is an integral part of the sediment transport processes. The resuspension of sediments from the cohesive bed follows the characteristic equation for resuspension of cohesive sediments, resulting in a certain mass flux of sediments into the water column. Resuspension of sediments from a noncohesive sediment bed, on the other hand, is based on the suspended load theory of van Rijn (1984; 1993). In both cases, the total mass of sediments resuspended into the water column is then apportioned between the fraction of cohesive and noncohesive sediments based on the respective fractions in the bed. Settling of cohesive sediments in the water column is modeled as a function of aggregation (flocculation) and settling. The effect of internal shear rates and water column concentrations on particle aggregation is implicitly defined in the settling velocity formulation. Noncohesive sediments, on the other hand, are assumed to settle discretely, without interaction with other particles. A unique characteristic of the model is its ability to use experimental results to describe parameters in the formulations of resuspension and deposition, including the effects of aggregation of cohesive sediment particles.

Sediments forming a cohesive sediment bed consolidate with time. A vertically segmented bed model incorporates the effect of consolidation on the sediment bed properties. Forcing functions such as time-varying sediment loads from river inflows, and concentrations of solids at open boundaries can be easily specified. Output from SED includes the spatial and temporal distribution of total suspended solids, water column concentrations of cohesive and noncohesive sediments, bed fractions of cohesive and noncohesive sediment, the mass of sediment deposited/eroded, and subsequent change in bed elevations.

## 6.2.1 Governing Equation

The three-dimensional advection-dispersion equation for transport of sediment of size class k (k = 1,2) is:

$$\frac{\partial C_{k}}{\partial t} + \frac{\partial UC_{k}}{\partial x} + \frac{\partial VC_{k}}{\partial y} + \frac{\partial (W - W_{s,k})C_{k}}{\partial z}$$

$$= \frac{\partial}{\partial x} \left( A_{H} \frac{\partial C_{k}}{\partial x} \right) + \frac{\partial}{\partial y} \left( A_{H} \frac{\partial C_{k}}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{H} \frac{\partial C_{k}}{\partial z} \right)$$
(6-1)

Boundary conditions:

$$K_H \frac{\partial C_k}{\partial z} = 0, z \to \eta$$
 (6-2a)



$$K_{H} \frac{\partial C_{k}}{\partial z} = E_{k} - D_{k}, z \rightarrow -H$$
 (6-2b)

where  $C_k$  = suspended sediment concentration of size class k (represented by 1 and 2, for cohesive and noncohesive sediments, respectively; u,v,w = velocity in the x, y and z-direction;  $A_H$  = horizontal diffusivity;  $K_H$  = vertical eddy diffusivity;  $E_k$ ,  $D_k$  = resuspension and deposition flux of size class k;  $\eta$  = water surface elevation above a specified datum; and H = bathymetric depth below the datum. Equation 6-1 is easily transformed to orthogonal curvilinear and sigma coordinates. When so done, it appears similar to Equation (3-55 and 3-56).

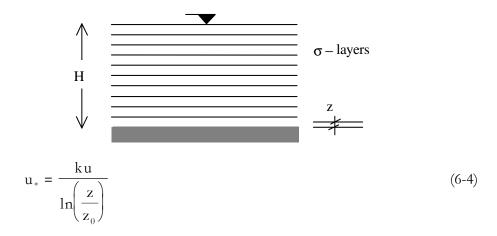
## 6.2.2 Bottom Shear Stress Computations

The bed shear stress is computed as follows:

$$\tau = \rho u_*^2 \tag{6-3}$$

where  $\rho$  = density of the suspending medium; and  $u_*$  = shear velocity.

For currents only, the shear velocity is defined by the Prandtl-von Karman logarithmic velocity profile



where  $k = von Karman constant \cong 0.40$ ; u = resultant near-bed velocity; <math>z = depth at the center of the bottommost layer; and  $z_0 = bottom$  friction specified as input to the model.

For wave-current induced bottom shear stress computations, the reader is referred to Section 7.2.

### 6.2.3 Resuspension of Cohesive Sediments



Laboratory experiments (Parchure and Mehta, 1985; Tsai and Lick, 1987; Graham et al., 1992) and field studies (Hawley, 1991; Amos et al., 1992) have revealed that only a finite amount of sediment can be resuspended from a cohesive sediment bed exposed to a constant shear stress as a result of armoring. The amount of fine-grained sediment resuspended from a cohesive sediment bed is given by Gailani et al. (1991) as:

$$\varepsilon = \frac{a_0}{T_d^m} \left( \frac{\tau_b - \tau_c}{\tau_c} \right)^n \tag{6-5}$$

where  $\varepsilon$ = resuspension potential (mg cm<sup>-2</sup>);  $a_0$ = constant depending upon the bed properties;  $T_d$  = time after deposition (days);  $\tau_b$ = bed shear stress (dynes cm<sup>-2</sup>);  $\tau_c$  = critical shear stress for erosion (dynes cm<sup>-2</sup>); and m, n = constants dependent upon the depositional environment.

The parameters in the above equation are generally determined from shaker studies (Tsai and Lick, 1987). Shaker studies have been conducted in at least twelve aquatic systems (Figure 6-1) and the data obtained from those studies have been used in a number of sediment transport modeling efforts (e.g., Ziegler and Nisbet, 1994; Lick et al., 1995; HydroQual, 1998).

Experimental results show that the total amount of sediment flux into the water column is not resuspended instantaneously but over a time period of approximately one hour (Tsai and Lick, 1987; MacIntyre et al., 1990). The resuspension rate is thus given by

$$E_{tot} = \frac{\varepsilon}{3600 \text{ seconds}}$$
 (6-6)

where  $E_{tor}$  is assumed to be constant until all available sediment is eroded. Once the amount  $\mathbf{\epsilon}$  has been resuspended,  $E_{tor}$  is set to zero until additional sediment is deposited and available for resuspension or until the shear stress increases (Gailani et al., 1991). The resuspension rate of sediments of class k ( $E_k$ ), which is needed in the governing equation, is then given by

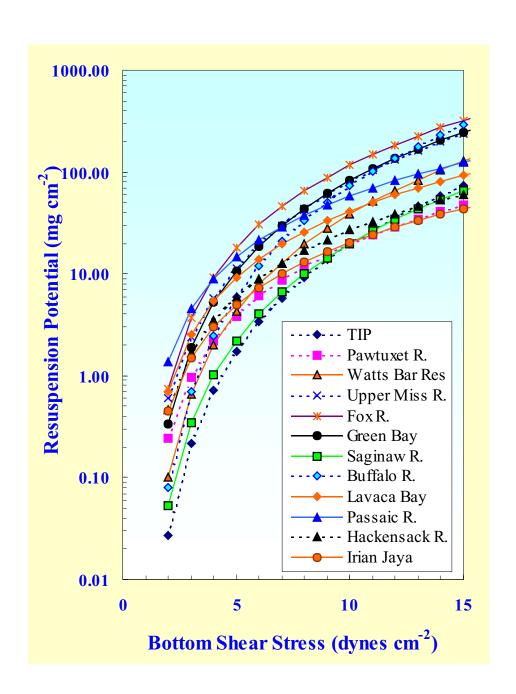
$$E_k = f_k E_{tot} (6-7)$$

where  $f_k$  = fraction of class k sediment in the cohesive bed.

## 6.2.4 Deposition of Cohesive Sediments

The cohesive nature of particles in suspension causes discrete particles to aggregate, forming flocs that vary in size and settling velocities. Variation in concentration and internal shear stress affects both the size and settling speed of the floc (Burban et al., 1990). Characterization of depositional fluxes in natural water systems can thus be







Resuspension potential as a function of bed shear stress for twelve different aquatic systems (based on shaker studies).

difficult. In SED, the deposition rate for cohesive sediments depends directly upon the sediment flux approaching the bed and the probability of the flocs sticking to the bed, according to the formulation of Krone (1962) as follows:

$$D_1 = -W_{s_1} C_1 P_1 \tag{6-8}$$

in which  $D_1$  = depositional flux (g cm<sup>-2</sup> s<sup>-1</sup>);  $W_{s,1}$  = settling velocity of the cohesive sediment flocs (cm s<sup>-1</sup>);  $C_1$  = cohesive suspended sediment concentration (g cm<sup>-3</sup>) near the sediment-water interface; and  $P_1$  = probability of deposition.

Settling speeds of cohesive flocs have been measured over a large range of concentrations and shear stresses (Burban et al., 1990). Experimental results show that the settling speed of cohesive flocs is dependent on the product of concentration and the water column shear stress at which the flocs are formed, resulting in the following relationship:

$$W_{s,1} = \alpha (C_1 G)^{\beta} \tag{6-9}$$

in which  $W_{s,1}$ ,  $C_1$ , and G are expressed in m day-1, mg L-1, and dynes cm-2, respectively. The above equation implicitly incorporates the effect of internal shear stress (G) on aggregation and settling. For saltwater suspensions, analysis of Burban et al. (1990) data revealed values of  $\alpha$  and  $\beta$  of 2.42 and 0.22, respectively. Figure 6-2 shows a comparison of Equation 6-9 using the above parametric values and Burban et al. data.

The water column shear stress (G) is computed from the hydrodynamic output (i.e., current velocity and vertical eddy viscosity) as follows:

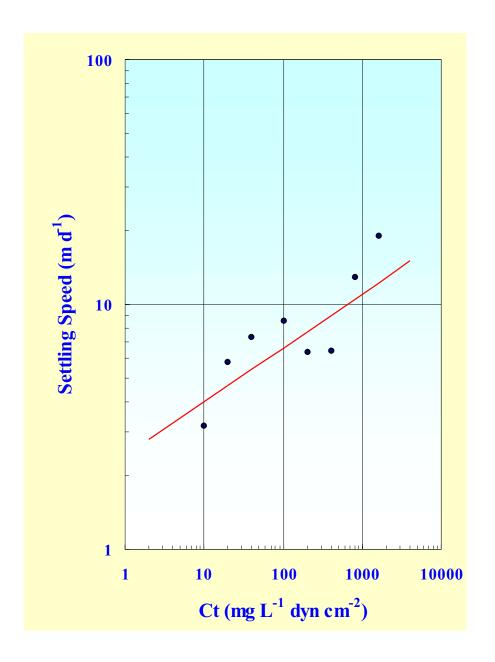
$$G = \rho K_M \left[ \left( \frac{\partial u}{\partial z} \right)^2 + \left( \frac{\partial v}{\partial z} \right)^2 \right]^{1/2}$$
 (6-10)

where  $K_M$  = vertical eddy viscosity, and  $\rho$  = density of the suspending medium.

The probability of deposition (P<sub>1</sub>) parameterizes the effects of floc size heterogeneity and near-bed turbulence on the deposition rate. The complex interactions occurring at the vicinity of the sediment-water interface cause only a certain fraction of settling sediments to actually become incorporated into the bed (Krone, 1962; Partheniades, 1992). Krone (1962) was the first to develop a relationship for the probability of deposition

$$\mathbf{P}_{1} = \begin{cases} 1 - \frac{\tau_{b}}{\tau_{d}}, & \tau_{b} \leq \tau_{d} \\ 0, & \tau_{b} > \tau_{d} \end{cases}$$
(6-11)







Settling speed function for cohesive sediments settling in saltwater compared to mean values of Burban et al., (1990) data.

where  $\tau_b$  = bottom shear stress (dynes cm<sup>-2</sup>), and  $\tau_d$  = critical shear stress for deposition (dynes cm<sup>-2</sup>). The above formulation has been incorporated into several cohesive sediment transport models including: STUDH (Ariathurai and Krone, 1976); TSEDH (Shrestha and Orlob, 1994); CSTM-H (Hayter and Mehta, 1986); and SEDZL (Ziegler and Nisbet, 1996). The critical shear stress for deposition ( $\tau_d$ ) is typically used as a calibration parameter in modeling studies because it is not well known. Limited experimental data indicate  $\tau_d$  ranges between 0.6 and 1.1 dynes cm<sup>-2</sup>, depending upon sediment concentration and type (Krone, 1962; Mehta and Partheniades, 1975). Partheniades (1992) developed an empirically based formulation that realistically represents the effects of variable floc size on probability of deposition. This can be expressed as:

$$P_{1} = 1 - \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{Y} e^{-\frac{\omega^{2}}{2}} d\omega$$
 (6-12)

where  $\omega$  = dummy variable, and

$$Y = 2.04 \log \left[ 0.25 \left( \frac{\tau_b}{\tau_{b,min}} - 1 \right) e^{1.27 \tau_{b,min}} \right]$$
 (6-13)

where  $\tau_{b,min}$  = bottom shear stress below which  $P_1$  = 1 (dynes cm<sup>-2</sup>).

The probability integral in Equation (6-12) can be accurately approximated by a cubic equation, yielding (for  $0 \le Y \le \infty$ ).

$$P_{1} = \frac{1}{\sqrt{2\pi}} e^{-\frac{y^{2}}{2}} \left( 0.4362z - 0.1202z^{2} + 0.9373z^{3} \right)$$
 (6-14)

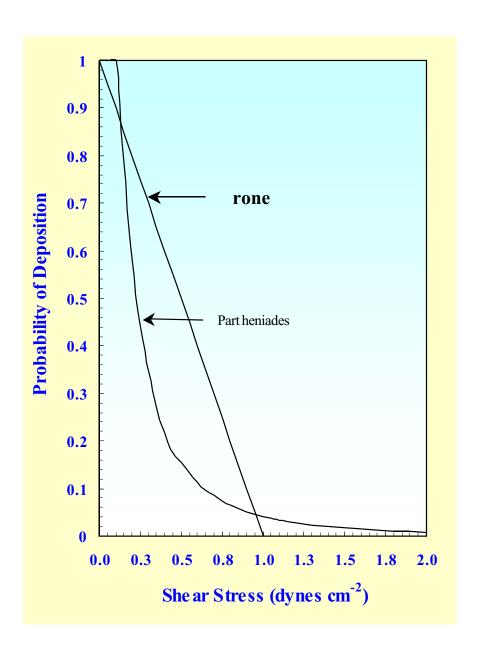
where:

$$z = (1 + 0.3327Y)^{-1}$$
 (6-15)

for 
$$Y < 0, P_1(-Y) = 1 - P_1(Y)$$

There are two primary differences between the Krone and Partheniades probability of deposition formulations as shown in Figure 6-3. First, the Partheniades approach results in significantly higher deposition than Krone's method in the low shear stress region, with  $P_1 = 1$  for shear stresses up  $\tau_{b,min}$ . Secondly, Partheniades' formulation allows finite deposition to occur, even for higher shear stresses.







Comparison of Krone (1962) and Parpheniades (1992) formulations for the probabilities of deposition of cohesive sediments.

## FIGURE 6-3

#### 6.2.5 Cohesive Sediment Bed Model

To realistically simulate the effects of sequential deposition and erosion, and the subsequent change in bed properties such as thickness and erodibility characteristics, a vertically segmented model of the cohesive sediment bed is constructed as shown in Figure 6-4. This is achieved by discretizing the sediment bed into seven layers. Each layer of the bed is characterized by a dry density  $(\rho_d)$ , a critical shear stress for erosion  $(\tau_{cr})$ , and an initial thickness. The "time after deposition" for each layer increases linearly from one day at the surface, which is composed of freshly deposited material, to seven days in the bottom layer. Previous laboratory results (Tsai and Lick, 1987; MacIntyre et al., 1990) have indicated that consolidation effects on resuspension are minimal after seven days of deposition, hence deposited sediments aged seven days or more are assumed to be seven days old. The resuspension potential equation shows that each layer decreases with time of consolidation ( $T_d$ ), in accordance with the ( $T_d$ )-m term. The layered bed model conserves mass, with resuspension and deposition fluxes occurring only at the bed level. During the course of a simulation, the bed model accounts for changes in thickness, the mass of cohesive and noncohesive sediments in each layer, resulting from resuspension and deposition at the sediment-water interface.

## 6.2.6 Resuspension of Noncohesive Sediments

The resuspension of sediment from a non-cohesive sediment bed is calculated using a procedure developed by van Rijn (1984). The van Rijn method has been shown to yield good results for predicting suspended load of fine sands (van Rijn, 1984; Garcia and Parker, 1991; van Rijn et al., 1993; Ziegler and Nisbet, 1994). Only a brief overview of the van Rijn method will be presented here, for details of the calculation procedure see van Rijn (1984). The first step in the procedure is to compare the bed-shear velocity  $u_*$  with the critical bed-shear velocity,  $u_*$  based on the local  $D_{50}$ , according to Shields criterion for initiation of motion. Suspended transport will only occur if the bed-shear velocity exceeds both the Shields criterion for bed load movement and the critical bed-shear velocity for suspension,  $u_*$  if resuspension does occur, the local  $D_{50}$  and bed-shear velocity,  $u_*$ , are used to determine the reference concentration at a height of z=a above the sediment bed,  $C_a$ . Finally, the local values of  $u_*$ ,  $D_{50}$  and  $C_a$  are used to calculate the suspended load transport rate.

Using the van Rijn method, the following procedure is adopted to calculate the suspended load transport.

#### 1. Compute the critical bed shear velocity for initiation of motion

A non-dimensional particle parameter is first introduced:



# Air-Water interface Water Depth **Bed Shear Stress** Layer No. $T_{d}$ I<sub>d</sub> cr (days) (dynes cm<sup>-2</sup>) Sediment-Water interface 1.0 1.0 2 2 3 3 1.0 Sediment Bed 4 4 1.0 1.0 5 5 6 6 1.0 4.0



Schematic of the sediment bed model.

### FIGURE 6-4

$$D_* = \left[ \frac{(s-1)g}{v^2} \right]^{1/3} D_{50}$$
 (6-16)

where s = specific gravity of the particles; g = gravitational acceleration;  $\upsilon$  = kinematic viscosity; and  $D_{50}$  = median particle diameter in the bed.

The critical bed shear velocity for initiation of bed motion is then computed using the Shields criteria as

$$u_{*,crbed} = [(s-1)gD_{50}\theta_{cr}]^{1/2}$$
 (6-17)

where  $\theta_{cr}$  = critical mobility parameter which is defined as

$$\begin{array}{lll} \theta_{cr} \! = \! 0.24 \ D_{*}^{-1} & D_{*} \leq 4 \\ \theta_{cr} \! = \! 0.14 \ D_{*}^{-0.64} & 40 < D_{*} \leq 10 \\ \theta_{cr} \! = \! 0.04 \ D_{*}^{-0.10} & 10 < D_{*} \leq 20 \\ \theta_{cr} \! = \! 0.013 \ D_{*}^{-0.29} & 20 < D_{*} \leq 150 \\ \theta_{cr} \! = \! 0.055 & D_{*} > 150 \end{array} \tag{6-18}$$

#### 2. Compute the critical shear velocity for resuspension

The critical shear velocity for resuspension is given by

$$\mathbf{u}_{*,\text{crsus}} = \mathbf{W}_{s,2} \tag{6-19}$$

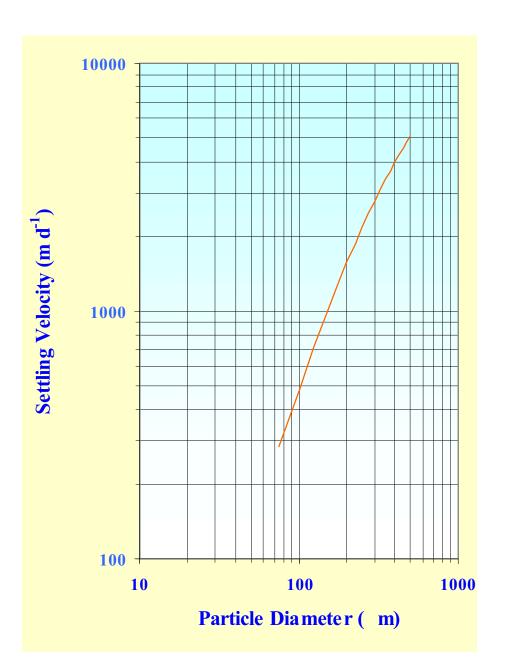
where  $W_{s,2}$  = settling velocity of the noncohesive suspended sediment. The settling velocity is specified as input to the model and is computed from the effective particle diameter ( $D_k$ ) of the suspended sediment using the formulation of Cheng (1997).

$$W_{s,2} = \frac{v}{D_k} \left[ \left( 25 + 1.2D_*^2 \right)^{0.5} - 5 \right]^{1.5}$$
 (6-20)

where  $D_*$  = non-dimensional particle parameter as shown in Eq.(6-16) with effective particle diameter  $D_k$ .

The dependence of  $W_{s,2}$  on  $D_k$  is illustrated in Figure 6-5, which shows that the settling speeds of suspended sand particles (i.e.,  $75 < D_k < 500 \mu m$ ) range from about 3,300 – 59,000  $\mu ms^{-1}$  (i.e.,  $\sim 280$  to 5,000 md<sup>-1</sup>).







Settling velocity as a function of particle diameter for noncohesive sediments (based on Cheng, 1997 formulation).

FIGURE 6-5

#### 3. Compute the bed shear velocity

The near-bed shear velocity due to the flow is computed as in Eq. (6-4).

$$u_* = \frac{ku}{\ln\left(\frac{z}{z_0}\right)} \tag{6-21}$$

#### 4. Suspended Load Transport

If the bed shear velocity  $(u_*)$  is less than the threshold for motion  $(u_{*,crbed})$  or less than the critical shear velocity for resuspension, then deposition occurs . If  $u_*$  exceeds  $u_{*,crbed}$  and  $u_{*,crsus}$ , the sediment flux is from the bed to the lower layer of the water column. The suspended load transport is then computed as follows:

Compute the transport stage parameter

$$T = \frac{u_*^2}{u_{*,crhed}^2} - 1 \tag{6-22}$$

Compute the reference level above bed

$$a = \max(0.01h, k_s)$$
 (6-23)

where h = water depth, and  $k_s = Nikuradse roughness height.$ 

$$C_{a} = \frac{0.015D_{k}T^{1.5}}{aD_{*}^{0.3}}$$
 (6-24)

where Ca is the reference concentration

Compute the β-factor

$$\beta = 1 + 2 \left(\frac{W_s}{u_*}\right)^2 \text{ for } 0.1 < \frac{W_s}{u_*} < 1$$
 (6-25)



Compute the  $\phi$ -factor

$$\phi = 2.5 \left(\frac{W_s}{u_*}\right)^{0.8} \left(\frac{C_a}{C_0}\right)^{0.4} \text{ for } 0.01 < \frac{W_s}{u_*} \le 1$$
 (6-26)

where  $C_0$  = maximum volumetric bed concentration = 0.65.

Compute the suspension parameter

$$\mathbf{Z'} = \mathbf{Z} + \phi = \frac{\mathbf{W_s}}{\beta \,\mathbf{ku_*}} + \phi \tag{6-27}$$

Compute the F-factor

$$F = \frac{\left(\frac{a}{h}\right)^{Z'} - \left(\frac{a}{h}\right)^{1.2}}{\left(1 - \frac{a}{h}\right)^{Z'} (1.2 - Z')}$$
(6-28)

Compute the suspended load transport

$$q_s = F z u C_a \tag{6-29}$$

where z = depth of the lowest  $\sigma$ -layer

#### Compute resuspension flux from the bed

The resuspension flux is calculated as the difference between the total suspended load transport (or the carrying capacity of the flow) and the existing horizontal sediment flux in the lowest  $\sigma$ -layer. If this difference is greater than zero, erosion occurs, whereas if the difference is less than zero, deposition occurs. It is therefore possible to have deposition even if  $u_*$  exceeds  $u_*$ <sub>crbed</sub> and  $u_*$ <sub>crsus</sub>.

In the model, resuspension is computed as

$$E = \frac{(\rho_s q_s - qzC_z)\Delta t}{\Delta x \Delta y}$$
(6-30)

where  $C_z$  = concentration of suspended sediment in the lowest  $\sigma$  layer;  $\rho_s$  is sediment particle density;  $\Delta t$  = time step; and  $\Delta x \Delta y$  = surface area of bottom.



#### 6.2.7 Deposition of Noncohesive Sediments

When the bed shear velocity  $(u_*)$  is less than the critical value  $(u_{*,crbed}$  or  $u_{*,crsus})$ , then the sediments in the water column deposit to the bed according to the formula:

$$D_2 = W_{s,2}C_2$$
 (6-31)

where  $D_2$  = noncohesive sediment depositional flux;  $W_{S,2}$  = settling velocity; and  $C_2$  = near-bed suspended sediment concentration.

## 6.2.8 Noncohesive Sediment Bed Armoring

An important assumption in the van Rijn procedure is that the bed sediments are homogeneous. A non-cohesive sediment bed is generally comprised of a wide range of particle sizes, from fine sands that are suspendable to coarse sands and gravels that are only transported as bed load. Bed armoring occurs when fine sands are eroded from a heterogeneous sediment bed and the coarser material that cannot be resuspended remains on the bed surface. During erosion, the suspendable sediments in the near-surface layer (referred to as the active layer) are depleted and a layer of coarse, non-suspendable sediments forms. Continuous depletion of suspendable sediments in the active layer will eventually reduce the erosion rate to zero, at which point the active layer is composed entirely of non-suspendable sediments, i.e., coarse sand and gravel. The sediment bed then becomes armored (Shen and Lu, 1983; Karim and Holly, 1986; van Niekerk et al., 1992).

The bed armoring process can be modeled by assuming that the sediment bed is composed of an active layer, which interacts with the water column, and a parent bed layer, which is below the active layer (Karim and Holly, 1986; van Niekerk et al., 1992). Resuspension of bed sediments is assumed to occur only from the active layer such that

$$E_2 = f_a E \tag{6-32}$$

where  $f_a$  = fraction of sediment in the active layer that is resuspendable; and E = resuspension rate for a homogeneous bed calculated using the van Rijn method. The fraction of resuspendable sediment in the parent bed  $(f_p)$  is determined from the initial grain size distribution data. The active layer thickness is determined using a modified form of the equation proposed by van Niekerk et al., (1992).

$$T_{a} = \frac{D_{50}\tau}{5\tau_{c50}} \tag{6-33}$$

where  $\tau$  = bed shear stress; and  $\tau_{c50}$  = critical shear stress necessary to initiate bed load motion for sediment with bed  $D_{50}$  and is calculated using Shields criteria. Changes in the composition of the active layer are made following the method of Karim and Holly (1986).



## 6.3 SEDZLJ Modeling Framework

The integration of SEDZLJ sediment transport routines into ECOMSED and other related code modifications provided four primary benefits to ECOMSED:

- 1. Computation of erosion fluxes as a function of measured erosion rates,
- 2. Division of total erosion fluxes into bedload and suspended load components,
- Simulation of bedload transport, and
- Simulation of a user-defined number of particle size classes.

These code modifications substantially improve the ability of ECOMSED to simulate the expected differential transport of sediments comprised of particles with a continuum of grain sizes and subject to significant bedload transport.

#### 6.3.1 Erosion

The governing equations for erosion in SEDZLJ (Jones and Lick, 2001) are:

$$E(\tau^{b}) = \left(\frac{\tau_{m+1} - \tau^{b}}{\tau_{m+1} - \tau_{m}}\right) E_{m} + \left(\frac{\tau^{b} - \tau_{m}}{\tau_{m+1} - \tau_{m}}\right) E_{m+1}$$
(6-34)

$$\ln E\left(T\right) = \left(\frac{T_0 - T}{T_0}\right) \ln E^{L+1} + \left(\frac{T}{T_0}\right) \ln E^{L} \tag{6-35}$$

where:  $E(\tau^b)$  = erosion rate as a function of shear stress ( $\tau$ );  $\tau^b$  = bottom shear stress;  $\tau_m$  = critical resuspension shear stress less than  $\tau^b$ ;  $\tau_{m+1}$  = critical resuspension shear stress greater than  $\tau^b$ ; E(T) = erosion rate as a function of depth in the sediment bed; T = sediment layer thickness;  $T_0$  = initial sediment layer thickness; and the superscripts L and L+1 denote depths in the sediment profile at the upper and low limits of the eroding sediment layer. Equations 6-34 and 6-35 can be combined to express the erosion rate as a function of both shear stress and depth. The onset of erosion is identified as the critical shear stress for erosion,  $\tau_{ce}$ , and is defined as the shear stress at which erosion is initiated at a rate of  $\tau_{ce}$ .

For non-cohesive particles, the critical shear stress for erosion can be estimated from the particle diameter as:



$$\tau_{ce} = \begin{cases} d & for \ d \le 400 \,\mu m \\ 4.14d & for \ d > 400 \,\mu m \end{cases}$$

$$(6-36)$$

#### 6.3.2 Non-Cohesive Bedload vs. Suspended Load Fractionation

When the shear stress acting on grains comprising the bed exceeds the critical shear stress for a given grain size, particles may be transported as bedload (in a thin layer in contact with the bed) or as suspended load (fully entrained in the water column away from the bed). The governing equations used to fractionate eroded sediments into bedload and suspended load are:

$$f_{SL} = \begin{cases} 0 & for \ \tau^{b} \leq \tau_{ce} \\ \frac{\ln(u_{*}/w_{s}) - \ln(\sqrt{\tau_{cs}/\rho_{w}}/w_{s})}{\ln(4) - \ln(\sqrt{\tau_{cs}/\rho_{w}}/w_{s})} & for \ \tau^{b} > \tau_{cs} \ and \ \frac{u^{*}}{w_{s}} < 4 \end{cases}$$

$$1 & for \ \frac{u_{*}}{w_{s}} > 4$$

$$(6-37)$$

$$\tau_{cs} = \begin{cases} \frac{1}{\rho_w} \left(\frac{4w_s}{d_*}\right)^2 & \text{for } d \le 400 \,\mu\text{m} \\ \frac{1}{\rho_w} \left(4w_s\right)^2 & \text{for } d > 400 \,\mu\text{m} \end{cases}$$

$$(6-38)$$

where:  $\tau_{ss}$  = critical shear stress for transport as suspended load;  $w_s$  = particle fall velocity;  $d_*$  = particle dimensionless diameter =  $d\left[\left(\rho_s - 1\right)g/v^2\right]$ ; d = particle diameter;  $\rho_s$  = particle density;  $f_{SL}$  = fraction of the total amount eroded that is transported as suspended load; and  $u_*$  = shear velocity. The fraction transported as bedload =  $(1-f_{SL})$ . Equations 6-37 and 6-38 can be used in



conjunction with the particle grain size distribution and critical shear stress for erosion to express the erosion flux of sediment by grain size that is transported by bedload and suspended load as a function of the bottom shear stress.

The bottom shear stress acting on the bed (*i.e.* the total bed shear stress) is a function of the total hydrodynamic roughness and can be expressed in terms of two separate components: (1) form roughness; and (2) grain roughness (*i.e.* skin friction). Individual grains on the surface of the sediment bed are subjected only to the skin friction component of the total bed shear stress. The total bed shear stress is computed from the near-bed hydrodynamic velocities according to the "log law" velocity profile:

$$u\left(z_{b}\right) = \frac{u_{*T}}{\kappa} \ln\left(\frac{z_{b}}{z_{0}}\right) \tag{6-39}$$

$$\tau_{T} = \rho \, u_{*T}^{2} = \rho \, C_{d} \, u \left( z_{b} \right)^{2} \tag{6-40}$$

$$C_d = \left(\frac{\kappa}{\ln \frac{z_b}{z_0}}\right)^2 \tag{6-41}$$

where:  $u(z_b)$  = near-bed flow velocity,  $u_{*T}$  = near-bed shear (friction) velocity;  $\kappa$  = von Karman constant = 0.4,  $z_b$  = height of the near-bed layer above the bed surface; and  $z_0$  = bed roughness height;  $\tau_T$  = total bed shear stress;  $\rho$  = density of the fluid; and  $C_d$  = coefficient of drag. In the sigma layer coordinate system of the hydrodynamic model,  $z_b$  is height above the bed at the mid-point of the bottom sigma layer.

The shear stress component associated with skin friction can be computed as a function of the total bed shear stress as follows (Grant and Madsen, 1982; Glenn and Grant, 1987):



$$u_{*s} = u_{*T} \left( \frac{\ln \frac{z_b}{z_0}}{\ln \frac{z_b}{z_{0s}}} \right) \tag{6-42}$$

$$\tau_{\scriptscriptstyle S} = \rho \, u_{\ast \scriptscriptstyle S}^{\ 2} \tag{6-43}$$

where:  $u_{*s}$  = the near-bed shear velocity attributable to skin friction; and  $z_{OS}$ = the roughness height of particles comprising the bed surface;  $\tau_s$  = the skin friction shear stress.

As part of the model development process, SEI and HydroQual verified that the SEDZLJ code was properly implemented in ECOMSED by simulating and successfully reproducing the laboratory results of Little and Mayer (1972).

#### 6.3.3 Bed Consolidation

Sanford's (2007) paper outlines in detail the overall theory behind the consolidation model implemented here. Essentially as cohesive sediments deposit or erode the density of the sediment bed changes in response to the addition or reduction of overlying sediment. The consolidation model reproduces the measured effects of changes in sediment bed properties at any point in the sediments as a function of overlying bed mass. Sanford (2007) also generally included the effects of bioturbation which is not implemented in this version of ECOMSED.

The basic premise of Sanford's model was to reproduce the changes in solids volume concentration ( $\phi_s$ ) and critical shear stress for erosion ( $\tau_c$ ) at a point due to changes in sediment bed structure. The parameter of interest ( $\phi_s$  or  $\tau_c$ ) is defined by an equilibrium profile which is generally described by the equation:

$$\phi_s = \phi_{\infty} - (\phi_{\infty} - \phi_{s0}) \exp(-cm)$$
(6-
44)

where  $\phi_{\infty}$  is the ultimate equilibrium value,  $\phi_{s0}$  is the surface value, m is the mass of the overlying sediment bed (can be converted to z with a density profile), and c is an empirically determined coefficient. The equilibrium profile is defined relative to the instantaneous sediment/water interface, so it moves with changes in the sediment bed height.

Once a sediment specific equilibrium profile has been determined, this can be applied to deposited layers in the sediment bed. At any point in time (t) and bed mass position (m), the instantaneous value of the property of interest is assumed to approach equilibrium in a first order manner.



$$\frac{\partial \phi_{s}}{\partial t} = r_{c} \left( \phi_{seq} - \phi_{s} \right) H \left( \phi_{seq} - \phi_{s} \right) - r_{s} \left( \phi_{s} - \phi_{seq} \right) H \left( \phi_{s} - \phi_{seq} \right) \tag{6-45}$$

where H is the Heaviside step function (H=1 when the argument is  $\geq 0$  and H=0 otherwise),  $r_c$  (1/day) is the empirically determined first order consolidation rate and  $r_s$  (1/day) is the empirically determined first order swelling rate.

The model structure above is mechanistically applied in SEDZLJ to deposited sediments. Sediments below a deposited layer, the parent bed, are assumed to retain field measured properties and not change. The consolidation model as implemented in SEDZLJ models the equilibrium profile of bulk density ( $\rho_b$ , g/cm<sup>3</sup>) instead of

 $\phi_s$ . Since  $\rho_b$  varies as a linear function of  $\phi_s$ , the overall mechanistic description remains unchanged. The reason for this change is because SEDZLJ is based on Sedflume measured erosion rates. Sedflume measured erosion rates (E) in consolidation experiments (Roberts et al., 1998) have been most accurately described with a power law formulation that is a function of applied shear stress ( $\tau$ ) and bulk density.

$$E = A\tau^n \rho_b^m \tag{6-46}$$

where A, n, and m are empirically determined coefficients. Additionally, an erosion rate threshold of 0.0001 cm/s is used in Sedflume to define the critical shear stress; therefore, it is a simple exercise to calculate critical shear stress for erosion  $(\tau_c)$  using the above equation with empirically determined coefficients and the known erosion rate.

$$\tau_c = \sqrt[n]{\frac{0.0001}{A\rho_b^m}} \tag{6-47}$$

With this information, the prediction of bulk density using the equilibrium profile and first order differential equation, the critical shear stress and erosion rate for any layer in the deposited sediments is easily calculated.

The above description is used for deposited beds in the cohesive size ranges. Sandy beds may also deposit. The bulk density of sands is assumed constant in the model at a value defined by the user. The mass of a sandy layer is still used mechanistically in Eq. 6-45 to determine the equilibrium density of layers below the sand, since the greater weight of the sandy layer will result in a higher degree of consolidation. The erosion properties of a deposited sandy layer are determined in an algorithm equivalent to the erosion properties of the sandy active layer in the SEDZLJ model [i.e. values are determined from Roberts et al., (1998) quartz data].



The following subroutines have been added for SEDZLJ with consolidation:

- · SJ\_SHUFFLE Incorporates a sub-grid into the SEDZLJ model to handle the consolidation of deposited material.
- SJ\_CONSOL Calculates equilibrium bulk density profile, the current bulk density for each sub-grid layer, and the resulting critical shear stress for that layer.



#### 7.0 Wave Module

#### 7.1 Introduction

Prediction of the wave dynamics is based on a parametric type wave model developed for this study in an orthogonal curvilinear coordinate system. The model is based on a Great Lakes Environmental Research Laboratory (GLERL) wave model developed by Donelan (1977) and modified by Schwab et al. (1984). This is a parametric type model based on the conservation of momentum applied to deep water waves (ratio of water depth to wave length greater than 0.5). The governing equations describe the local momentum balance rather than the transport of energy. The momentum input to the model results from drag on the waves, which depends on the wave height and the differential speeds between the wave and the wind. An important feature of this model is the provision for a "fossil" wave field that may be left behind by a rapidly changing wind (Schwab et al., 1984). The model determines its computational time step dynamically based on the maximum winds for each hour. Given a description of the coastal bathymetry and a two dimensional, time-dependent wind field, the model predicts significant wave heights, wave periods, and wave directions.

The original GLERL model has successfully been applied to Lake Michigan (Liu et al., 1984) and Lake Erie (Schwab et al., 1984). It is also being used in the Great Lakes Coast Watch program. Additional application of the model in an estuarine environment includes the study on the prediction of waves in Chesapeake Bay (Lin et al. 1999). The model has also been compared against four currently available and well-recognized wave models (ACES, HISWA, WAVD and SWAN described by Leenknecht et al. (1992), Booij and Holthuijsen (1995), Resio and Perrie (1989) and Holthuijsen et al. (1993), respectively. The GLERL model performed quite well in simulating the wave field generated by tropical storm Danielle over northern Chesapeake Bay in September 1992. It gave the best prediction of significant wave height and showed a good response to a sharply turning wind.

The current wave model differs from the original GLERL model in two ways. First, the wave model is transformed to a curvilinear coordinate system to take advantage of the orthogonal curvilinear grid of the ECOM hydrodynamic model used in the present study. Second, it incorporates the frictional effect on the wave as it moves into shallower water.

The formulation of the wave prediction model is based on the assumption that the potential and kinetic energies are equally partitioned and that the deep water linear wave theory applies such that the group velocity is one half the phase speed. The transformation of the wave momentum equation into an orthogonal curvilinear coordinate system ( $\xi_1$ ,  $\xi_2$ , z) as shown in Figure 7-1, yields the following momentum conservation equations:

$$\frac{\partial \mathbf{M}_{\xi_{1}}}{\partial t} + \frac{1}{\mathbf{h}_{1}\mathbf{h}_{2}} \left[ \frac{\partial \left(\mathbf{h}_{2}T_{\xi_{1}\xi_{1}}\right)}{\partial \xi_{1}} + \frac{\partial \left(\mathbf{h}_{1}T_{\xi_{1}\xi_{2}}\right)}{\partial \xi_{2}} \right] = \frac{\tau_{\xi_{1}}^{w}}{\rho_{w}}$$
(7-1)



$$\frac{\partial \mathbf{M}_{\xi_2}}{\partial t} + \frac{1}{\mathbf{h}_1 \mathbf{h}_2} \left[ \frac{\partial (\mathbf{h}_2 \mathbf{T}_{\xi_1 \xi_2})}{\partial \xi_1} + \frac{\partial (\mathbf{h}_1 \mathbf{T}_{\xi_2 \xi_2})}{\partial \xi_2} \right] = \frac{\tau_{\xi_2}^{w}}{\rho_w}$$
(7-2)

The momentum components  $\mathrm{M}_{\boldsymbol{\xi}_1}$  and  $\mathrm{M}_{\boldsymbol{\xi}_2}$  are defined as

$$M_{\xi_{I}} = g \int_{0}^{\infty} \int_{0}^{2\pi} \frac{F(f,\theta)}{C(f)} \cos\theta \, d\theta \, df \tag{7-3}$$

and

$$\mathbf{M}_{\xi_2} = g \int_0^\infty \int_0^{2\pi} \frac{\mathbf{F}(\mathbf{f}, \theta)}{\mathbf{C}(\mathbf{f})} \sin\theta \, d\theta \, d\mathbf{f} \tag{7-4}$$

Here  $F(f,\theta)$  is the wave energy spectrum as a function of frequency (f) and direction ( $\theta$ ) and C(f) is the phase speed.  $\tau_{\xi_1}$  and  $\tau_{\xi_2}$  are wind stress along  $\xi_1$  and  $\xi_2$  directions,  $\rho_w$  is the density of air.

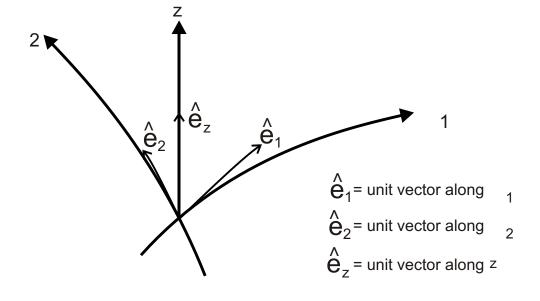
The wave momentum flux  $T_{\xi_1\xi_1}$ ,  $T_{\xi_1\xi_2}$ , and  $T_{\xi_2\xi_2}$ , are defined as follows:

$$T_{\xi_1 \xi_1} = \frac{g}{2} \int_0^\infty \int_0^{2\pi} F(f, \theta) \cos^2 \theta \ d\theta \ df \tag{7-5}$$

$$T_{\xi_1 \xi_2} = T_{\xi_2 \xi_1} = \frac{g}{2} \int_0^\infty \int_0^{2\pi} F(f, \theta) \sin \theta \cos \theta d\theta df$$
 (7-6)

$$T_{\xi_2 \xi_2} = \frac{g}{2} \int_0^\infty \int_0^{2\pi} F(f, \theta) \sin^2 \theta d\theta df$$
 (7-7)







Curvilinear coordinate system.

FIGURE 7-1

Considering the wave energy is distributed about the mean angle  $\theta_0$  as cosine square and there is no energy for  $|\theta - \theta_0| > \pi/2$ ,

$$F(f, \theta) = \frac{2}{\Pi} E(f) \cos^2 (\theta - \theta_o)$$
 (7-8)

Here E(f) is the spectral wave energy.

If  $\theta_0$  is independent of frequency, the momentum fluxes may be expressed in terms of  $\theta_0$  and the variance as:

$$\sigma^2 = \int_0^\infty E(f) df$$
 (7-9)

Integration of Equations 7-5 to 7-7 results

$$T_{\xi_1 \xi_1} = g \left( \frac{\sigma^2}{4} \cos^2 \theta_0 + \frac{\sigma^2}{8} \right) \tag{7-10}$$

$$T_{\xi_1 \xi_2} = T_{\xi_2 \xi_1} = g \left( \frac{\sigma^2}{4} \cos \theta_0 \sin \theta_0 \right)$$
 (7-11)

$$T_{\xi_2 \xi_2} = \left( g \frac{\sigma^2}{4} \sin \theta_0 + \frac{\sigma^2}{8} \right) \tag{7-12}$$

It is interesting to note here that Equations 7-10 to 7-12 expressing the momentum flux are independent of the spectral shape. Moreover,  $\sigma^2/8$  in Equations 7-10 and 7-12 represents an isotropic term, which causes a wave pressure gradient from areas of high waves toward areas of low waves.

The relation between the variance  $\sigma^2$  and the momentum components in Equations 7-1 and 7-2 can be obtained by fitting all fetch-limited frequency spectra to JONSWAP function (Hasselmann et al., 1975):

$$E(f) = \alpha g^{2} (2\Pi)^{-4} f^{-5} \exp \left\{ -\frac{5}{4} \left( \frac{f}{f_{p}} \right)^{-4} \right\} \cdot \left\{ 3.3^{\exp \left[ -\frac{(f - f_{p})^{2}}{2\beta^{2} f_{p}^{2}} \right]} \right\}$$
 (7-13)

$$\beta = 0.07, \text{ for } \qquad \qquad f \leq f_{_{\! F}}$$
 
$$\beta = 0.09, \text{ for } \qquad \qquad f > f_{_{\! F}}$$



Two scale parameters  $f_p$  and  $\alpha$  are peak frequency and the Phillips constant respectively. Donelan (1977) suggested an empirical relation between these two parameters which successfully eliminates the dependency on the fetch length described in the original JONSWAP formula. This relations is as follows:

$$\alpha = 0.0097 \left(\frac{U}{C_p}\right)^{\frac{2}{3}}$$
 (7-14)

Here  $C_p = g/2\pi f_p$  and U is wind speed 10 m above sea level.

Integrating equation 7-13 and 7-14 yields

$$\frac{\sigma^2}{|\mathbf{M}|} = \frac{C_p}{g} \tag{7-15}$$

and

$$\sigma^{2} = 0.30\alpha g^{2} (2\pi)^{-4} f_{p}^{-4}$$
 (7-16)

Here |M| is the magnitude of momentum vectors  $M_{\xi_1}$  and  $M_{\xi_2}$ .

Now the numerical solution is sought to solve equations 7-1, 7-2 (substituting equation 7-10 to 7-12) for variance ( $\sigma^2$ ), wave period ( $T = \frac{2\pi}{f_p}$ ) and direction  $\theta$ . The significant wave height,  $H_s$ , is then computed using the following relation.

$$H_{s} = 4\sigma \tag{7-17}$$

#### 7.2 Wave Induced Bottom Shear Stress

Bed shear stresses due to currents and waves are crucial for calculating sediment resuspension and deposition fluxes (Fredsoe and Deigaard, 1991; van Rijn, 1993). This stress is generally higher than that induced by currents computed by hydrodynamic processes (Grant and Madsen, 1979; Glenn and Grant, 1987). Hydrodynamic models are based on processes with much longer time scales. Wind waves, on the other hand, are high frequency short waves. These waves are generally considered deep water waves, represented as governing equations (USCOE, 1984; Fredsoe and Deigaard, 1991) which are different than the shallow water wave equations. The computation of bottom shear stress due to wave induced currents is presented below.

The hydrodynamic model provides the near bottom current velocity (U), direction of current ( $\theta_c$ ), and the total water depth (h). The wave model predicts the significant wave height (H<sub>s</sub>), period (T) and direction ( $\theta$ ). Linear wave theory is used to translate the wave parameters (H<sub>s</sub> and T) into a near-bed peak orbital velocity (U<sub>p</sub>) and peak orbital amplitude (A<sub>p</sub>) as follows



$$U_{p} = \frac{\pi H_{s}}{T \sinh\left(2\pi \frac{h}{L}\right)}$$
(7-18)

$$A_{p} = \frac{H_{s}}{2 \sinh\left(2\pi \frac{h}{L}\right)}$$
(7-19)

where the wave length (L) is given by

$$L = C_{o}T \tag{7-20}$$

and the shallow water wave speed (C<sub>o</sub>) is

$$C_o = \sqrt{g h} \tag{7-21}$$

in which g is the gravitational acceleration.

The Grant-Madsen wave-current model (Grant and Madsen, 1979; Glenn and Grant, 1987) is then used to calculate bottom shear stresses due to currents and waves. Inputs to the model are:

U = magnitude of the near bottom current velocity

 $\Phi = \theta$ . the difference between wave and current direction

 $U_p$  = near-bed peak orbital velocity  $A_p$  = near-bed peak orbital amplitude  $z_0$  = effective bottom roughness height

Output from the model is the bottom shear velocity ( $u_*$ ). The bed shear stress ( $\tau_b$ ) is then computed as

$$\tau_b = \rho \ u_*^2 \tag{7-22}$$

where  $\rho$  = density of water. In the absence of wave,  $u_*$  is a function of U only. The details of bed shear stress computations without wave and current interaction can be found in Blumberg and Mellor (1987).

Surface wind waves can significantly increase bed shear stresses as pointed out in previous studies (Fredsoe and Deigaard, 1991; van Rijn, 1993). The magnitude of the bed shear stress is a function of the characteristics of wind wave field, which is highly variable in time. Bed shear stresses due to the combined effects of waves and currents can result in stresses that are two orders of magnitude higher than stresses resulting from currents alone. These higher stresses may result in significantly different bed erosion and sediment transport. Therefore, effects of wind generated waves may be an important mechanism that should be included in the current modeling framework.



#### 8.1 Finite Difference Formulation

The governing equations form a set of simultaneous partial differential equations which cannot be solved using known analytic methods. The equations require numerical computational methods using discretized equations on a grid. In anticipation of constructing the finite differencing scheme, the governing equations have been cast into their flux form. This is to insure that certain integral constraints are maintained by the differencing.

### 8.1.1 Finite Differencing

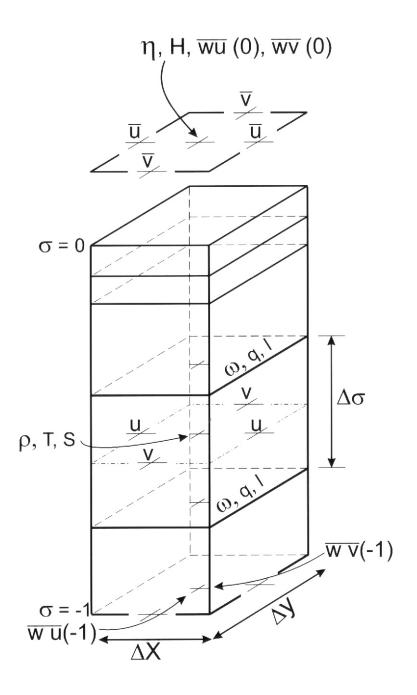
The relative positions of the variables on the staggered computation "C" grid are shown in Figure 8-1. The staggered arrangement uses U at points to the east and west of the point where  $\eta$  and H are defined and V at points to the north and south of the  $\eta$  and H points. This type of grid has been shown by Batteen and Han [1981] to be the most effective grid for high resolution models. The  $\Delta x$  and  $\Delta y$  are the constant horizontal grid spacings and  $\Delta \sigma$  is the vertical increment which varies in thickness to accommodate more resolution near the surface and bottom.

The finite difference equations used in ECOM can be demonstrated to be of second order accuracy in space and time and to conserve energy, temperature, salinity, mass, and momentum. Finally, the model's computer code has been deliberately designed to be economical on modern array processing computers.

## 8.1.2 Subgrid Scale Parameterizaton

Horizontal mixing coefficients for both momentum and heat/salinity are used to parameterize all processes which are not resolved on the numerical grid. Typically, these mixing coefficients are chosen such that they are sufficient to provide minimal smoothing without excessive damping of real oceanographic processes. Since the numerical grid can be non-uniform, the mixing coefficients must vary proportionally in order to maintain a uniform grid Reynolds number. The parameterization suggested by Smagorinsky (1963), which also depends on the horizontal grid spacing, has been used in the model.







The locations of the variables on the finite difference grid.

## FIGURE 8-1

The terms related to small-scale mixing processes not directly resolved by the model are parameterized as horizontal diffusion as described in Equations (3-39) and (3-44) and calculated according to Smagorinsky 91963):

$$A_{M} = \alpha \Delta x \Delta y \left[ \left( \frac{\partial U}{\partial x} \right)^{2} + \left( \frac{\partial V}{\partial y} \right)^{2} + \frac{1}{2} \left( \frac{\partial U}{\partial y} \right) + \left( \frac{\partial V}{\partial x} \right)^{2} \right]^{1/2}$$
(8-1)

and where the notation is based upon Cartesian coordinates and variable names are those used conventionally. The parameter  $\alpha$  is typically equal to 0.10 and has ranged from 0.01 to 0.5 in various applications. Here  $A_H = A_M$ , but the code has provisions to relax this constraint

#### 8.1.3 Stability Constraints

The leap-frog differencing used for the time stepping introduces a tendency for the solution at even and odd time steps to split. This time splitting is removed by a weak filter [Asselin, 1972] where the solution is smoothed at each time step according to

$$F_{s}^{n} = F^{n} + \frac{\alpha}{2} \left( F^{n+1} - 2F^{n} + F_{s}^{n-1} \right)$$
 (8-2)

where  $\alpha = 0.05$  and  $F_s$  is a smoothed solution.

This technique introduces less damping than either the Euler-backward or forward stepping techniques.

The Courant-Friedrichs-Levy (CFL) computational stability condition on the vertically integrated, external mode, transport equations limits the time step as shown by Blumberg and Mellor [1981a] according to

$$\Delta t \le \frac{1}{C_t} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right)^{-1/2} \tag{8-3a}$$

where

$$C_t = 2(gH)^{1/2} + \overline{U}_{max}$$
 (8-3b)

Ūmax is the maximum average velocity expected. There are other restrictions but in practice the CFL limit is the most stringent. The model time step is usually 90% of this limit. The internal mode has a much less stringent time step since the fast moving external mode effects have been removed. The time step criteria is analogous to the one for the external mode given above and is

$$\Delta T \le \frac{1}{C_T} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right)^{-1/2} \tag{8-4}$$



where  $C_T = 2C + U_{max}$ , with C being the maximum internal gravity wave speed commonly of order 2 m/s and  $U_{max}$  is the maximum advective speed. For typical coastal ocean conditions the ratio of the time steps,  $\Delta T/\Delta t$ , is often a factor of 3-100.

Diffusion is important in the internal mode but does not affect the overall choice of time step, unless the grid Reynolds number is of order 1, in which case

$$\Delta T < \frac{1}{4A_H} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right)^{-1} \tag{8-5}$$

must be used.

A rotational condition is

$$\Delta t < \frac{1}{f} = \frac{1}{2\Omega \sin \theta} \tag{8-6}$$

where  $\Omega$  is the angular velocity of the earth and  $\theta$  is the latitude. However, even for high latitudes the rotational condition is not a limiting factor.

#### 8.2 Advection Algorithms

Accurately simulating the transport of salinity, temperature, sediment and tracers can be difficult, particularly in hydrodynamic and sediment transport problems involving the propagation of steep gradients, or fronts. In estuarine and coastal problems, the propagation of fronts is important, particularly in the zone where freshwater and saltwater mix. Three algorithms, each of which may provide distinct advantages for a particular problem, are available for use in ECOMSED: central difference, upwind difference and the Multidimensional Positive Definite Advection Transport Algorithm (MPDATA).

The central difference algorithm is second-order accurate, generates no numerical diffusion and is computationally efficient. However, this method is not positive definite and negative salinities/temperatures/sediment concentrations, which are physically impossible, may be generated in certain types of hydrodynamic and sediment transport problems. In addition, numerical ripples may be generated ahead of and behind fronts. Upwind differences are only first-order accurate and may introduce significant numerical diffusion into a solution depending upon typical current speeds and grid sizes. An advantage of upwind transport is that the algorithm is positive definite and the most computationally efficient of any of the advective schemes.

An improvement over both the central and upwind methods, particularly with regard to the transport of fronts, is MPDATA, which is described in detail by Smolarkiewicz (1984), Smolarkiewicz and Clark (1986) and Smolarkiewicz and Grabowski (1990). The general concept used in MPDATA is the successive application of an upwind transport algorithm, which is first-order accurate and positive definite, such that numerical diffusion, generated by a first-order truncation error, is minimized. A correction to the first-order truncation error is made by reapplying the upwind algorithm, after the initial upwind step, using an "anti-diffusion" velocity that is based on the local first-order truncation error. The corrective step may be applied an arbitrary number of times, resulting in a successive reduction in the numerical diffusion generated by the initial upwind step. This procedure yields an advection algorithm that is second-order accurate, and positive definite. Furthermore, MPDATA preserves the local monotone character of the advection field, such that,



the field is free of numerically-generated ripples, provided that the anti-diffusion velocities are property bounded. The greatest drawback to routine use of MPDATA is its large demand for computational resources. The execution time for a typical simulation can double the time required for a case involving central or upwind differences. On vector computers this factor is even larger because of the unavoidable many "IF" statements needed in the computer code.

#### 8.3 Thin Dams

The model can be configured to represent thin obstructing structures such as groins, wave breakers, or dams. No flow exchange will be allowed between two grid cells separated by these thin dams. This feature is particularly useful to model harbor facilities where flow around thin and elongated man-made structures needs to be modeled without masking out grid cells. Designation of thin dam follows the same conventions for computational variables shown in Figure 8-1.

## 8.4 Semi-Prognostic Density Computations

When the model is configured with climatological temperature and salinity data and run in prognostic mode, often times model computation becomes unstable over time. This is mainly due to departures of initial temperature and salinity in prognostic computations which were caused by internal mixing, bottom friction, and flows across steep bathymetric slope along the open water boundaries. Nevertheless, this is mainly due to the insufficient boundary information prescribed along the boundary locations. The sea level fluctuations induced by density and weather related events are absent from the input data. The combined effect of insufficient sea level boundary conditions and dynamic density field, which is not supported by computed and prescribed temperature and salinity boundary conditions, induces artificial noise along the boundary cells and eventually causes model to crash. In order to solve these problems, a numerical technique suggested by Sheng et. al.(2001) was implemented. This procedure is equivalent to adding a forcing term to the momentum equations by modifying the horizontal pressure gradient term seen by the model (Sheng et. al, 2001).

In order to solve the pressure gradients over depth, the equation becomes.

$$\frac{\partial \mathbf{p}}{\partial \mathbf{z}} = \left[\alpha \rho_{\rm m} + (1 - \alpha) \rho_{\rm d}\right] \mathbf{g} \tag{8-7}$$

p = pressure

 $\rho_{\rm d}$  = Initial T/S derived from data

 $\rho_{m}$  = Model computed T/S

 $\alpha$  = coefficient (0 to 1) If  $\alpha$  = 1, pure prognostic. If  $\alpha$  = 0, pure diagnostic.

The equation denotes that the model solution adjusts its pressure gradients with initially specified density field( $\rho_d$ ) and computed density( $\rho_m$ ).

#### 8.5 Empirical Vertical Turbulent Mixing

The Mellor-Yamada turbulence model can yield accurate hydrodynamic simulations. However, use of this approach typically requires using about 10 levels in the vertical. For many problems, this level of vertical resolution is impractical, due to constraints on data, time or budget. Another method to simulate the effects of turbulence on vertical mixing processes is use of an empirical formula. This approach can be quite useful



for problems that require use of low vertical resolution.

The empirical vertical mixing theory is based on ideas of Kent and Pritchard (1959) and Officer (1976). There are two adjustable coefficient  $\alpha$  and  $\beta$  which set the amount of mixing at a location. They can be thought of as proportional to the bottom roughness. They are unitless scaling factors.

$$\mathbf{K}_{\mathbf{M}} = \mathbf{K}_{\mathbf{0}} \left( 1 + \beta \, \mathbf{R}_{\mathbf{i}} \right)^{-1} \tag{8-8}$$

$$K_{H} = K_{o} (1 + \beta R_{i})^{-2}$$
 (8-9)

with

$$K_{o} = \alpha Z^{2} \left( 1 + \frac{z}{D} \right)^{2} \left[ \left( \frac{\partial u}{\partial z} \right)^{2} + \left( \frac{\partial v}{\partial z} \right)^{2} \right]^{1/2}$$
(8-9a)

$$R_{i} = -\frac{\frac{g}{\rho} \frac{\partial \rho}{\partial z}}{\left(\frac{\partial u}{\partial z}\right)^{2} + \left(\frac{\partial v}{\partial z}\right)^{2}} = \frac{\text{buoyancy}}{\text{shear}}$$
(8-9b)

Note: turbulent Prandtl number is

$$Pr = \frac{K_{H}}{K_{M}} = \frac{1}{1 + \beta R_{s}}$$
 (8-9c)

Several test simulations with stratified conditions suggest that the values of  $0.01 \sim 1.0$  for coefficient  $\alpha$  and  $0.1 \sim 1.0$  for  $\beta$  can be used. However, it is advised to experiment with sufficient ranges of  $\alpha$  and  $\beta$  for the sensitivity in a particular model application.

#### 8.6 netCDF Output Format

ECOMSED has utilized universally accepted network compatible data format (netCDF) for its output. This data format is portable to any computer systems. Many utility programs are available in scientific community.

## 8.7 Flooding and Drying

A physical feature of flooding and drying of tidal flats based upon Flather and Heaps (1975) has been incorporated into ECOMSED. The treatment is based on both total water depth (D = H + h) and elevation gradient with adjacent grid cells. For implementation of the flooding and drying scheme, a minimum threshold depth (Dmin) and a critical elevation gradient (e) are pre-assigned (via model input). Figure 8-2 illustrates ECOMSED grid conventions. At each external computational timestep, Di,j, Di+1,j and Di,j+1 are checked (Figure 7-2). The procedure to determine whether a grid cell is either "wet" or "dry" is illustrated



in Figure 8-3 (Kim, 1999) and depends upon whether the D and elevation gradient (Dh) are greater or less than Dmin and e, respectively. A land cell is always "dry" and a water cell can be "wet" or "dry". To insure that a water cell is always "dry", the cell can be initialized with a large negative value of H or can be pre-defined as a land cell. But for the conservation of mass and momentum, ECOMSED requires a non-zero water depth be specified (initialized) in the model domain.



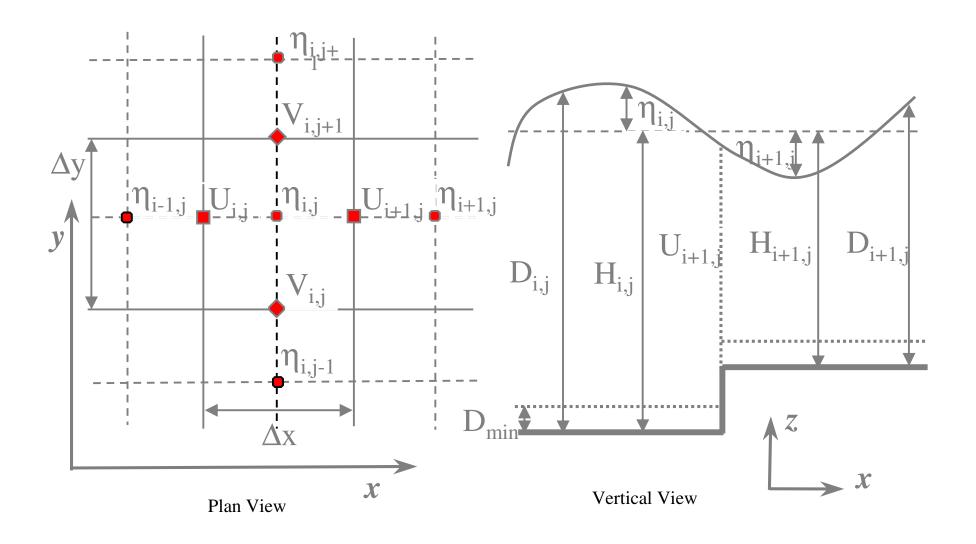
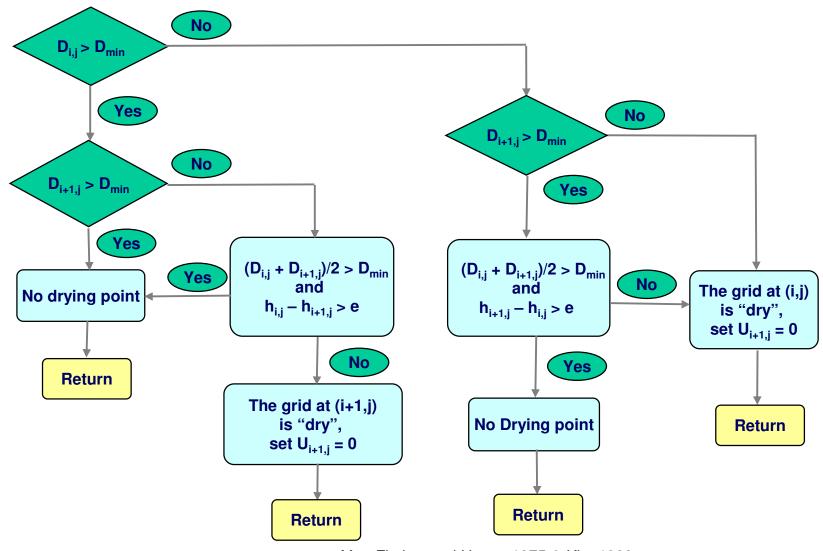


Figure 8-2. Schematic illustration of the ECOMSED Grid



After Flather and Heaps 1975 & Kim 1999

Figure 8-3. Flow chart of wetting/drying scheme

# 9.0 Structure of Computer Code

## 9.1 Fortran Symbols

The FORTRAN symbols followed by their corresponding analytical symbols in parentheses and a brief description of the symbols are listed in Table 9-1.

$ \begin{matrix} I, J \ (i,j) \\ IM, JM \\ Outer limits of 1 and J \\ K \ (k) \\ Vertical grid index; K = 1 at the top and K = KB at the bottom INT internal mode time step index external mode time step index external mode time step index [EXT]                                    $	Indices	Description
K (k) vertical grid index; K = 1 at the top and K = KB at the bottom internal mode time step index external mode time step index  Constants	I, J (i,j)	horizontal grid indexes
INT internal mode time step index external mode time step index  Constants  DTE $(\Delta t_E)$ external mode time step, (s) DTI $(\Delta t_I)$ internal mode time step, (s) EXTINC short wave radiation extinction coefficient, $(m^{-1})$ HORCON(C) the coefficient of the Smagorinsky diffusivity IEND total internal model time steps IPRINT the interval in IINT at which variables are printed ISPLIT DTI/DTE  MODE if $MODE = 2$ , a 2-D calculation is performed if $MODE = 3$ , a 3-D prognostic calculation is performed if $MODE = 3$ , a 3-D approachis calculation is performed if $MODE = 4$ , a 3-D diagnostic calculation is performed inverse, horizontal, turbulence Prandtl number  TR short wave surface transmission coefficient UMOL background vertical diffusivity  One-dimensional Arrays  Z(0) sigma coordinate which spans the domain, Z = 0 (surface) to Z = -1 (bottom) sigma coordinate, intermediate between Z  DZ( $\delta coordinate = 2$ ) $E(K) - E(K + 1)$ $E(K) - E($	IM, JM	outer limits of I and J
	K (k)	vertical grid index; K = 1 at the top and K = KB at the bottom
	INT	internal mode time step index
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EXTINC short wave radiation extinction coefficient, (m¹) HORCON(C) the coefficient of the Smagorinsky diffusivity total internal model time steps IPRINT the interval in IINT at which variables are printed ISPLIT DTI/DTE  MODE if MODE = 2, a 2-D calculation is performed if MODE = 3, a 3-D prognostic calculation is performed if MODE = 4, a 3-D diagnostic calculation is performed if MODE = 4, a	,	
$\begin{array}{lll} \mbox{HORCON(C)} & \mbox{the coefficient of the Smagorinsky diffusivity} \\ \mbox{IEND} & \mbox{total internal model time steps} \\ \mbox{IPRINT} & \mbox{the interval in IINT at which variables are printed} \\ \mbox{ISPLIT} & \mbox{DTI/DTE} \\ \mbox{MODE} & \mbox{if MODE} = 2, a 2-D calculation is performed} \\ \mbox{if MODE} = 3, a 3-D prognostic calculation is performed} \\ \mbox{if MODE} = 4, a 3-D diagnostic calculation is performed} \\ \mbox{RFE, RFW, RFN, RFS} & 1 or 0 on the four open boundaries; for use in BCOND} \\ \mbox{SMOTH} (\alpha) & parameter in the temporal smoother} \\ \mbox{TPRNI } (A_{H}/A_{M}) & inverse, horizontal, turbulence Prandtl number} \\ \mbox{TR} & short wave surface transmission coefficient} \\ \mbox{UMOL} & background vertical diffusivity} \\ \mbox{One-dimensional Arrays} \\ \mbox{Z(o)} & sigma coordinate which spans the domain, Z = 0 (surface) to Z = -1 (bottom)} \\ \mbox{ZZ} & sigma coordinate, intermediate between Z} \\ \mbox{DZ}(\delta\sigma) & = Z(K)-Z(K+1) \\ \mbox{DZZ} & = ZZ(K)-ZZ(K+1) \\ \mbox{Two-dimensional Arrays} \\ \mbox{AAM2D} & vertical average of AAM (m^2s^{-1})} \\ \mbox{ART, ARU, ARV} & cell areas centered on the variables, T, U and V respectively (m^2)} \\ \mbox{ADVUA, ADVVA} & sum of second, third and sixth terms in equations (3-46, 3-47)} \\ \mbox{ADX2D, ADY2D} & vertical integrals of ADVX, ADVY} \\  \end{array}$		
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Two-dimensional Arrays  AAM2D vertical average of AAM (m²s⁻¹)  ART, ARU, ARV cell areas centered on the variables, T, U and V respectively (m²)  ADVUA, ADVVA sum of second, third and sixth terms in equations (3-46, 3-47)  ADX2D, ADY2D vertical integrals of ADVX, ADVY	$DZ(\delta\sigma)$	= Z(K)-Z(K+1)
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ADVUA, ADVVA sum of second, third and sixth terms in equations (3-46, 3-47) vertical integrals of ADVX, ADVY		
ADX2D, ADY2D vertical integrals of ADVX, ADVY		
·		
COR(f) the Coriolis parameter (s <sup>-1</sup> )	COR(f)	the Coriolis parameter (s <sup>-1</sup> )
CURV2D the vertical average of CURV	( )	·



Table 9-1. Fortran Symbols (Cont.)

Indices	Description
DUM	Mask for the $u$ component of velocity; = 0 over land; =1 over water
DVM	Mask for the v component of velocity; = 0 over land; =1 over water
FSM	Mask for scalar variables; = 0 over land; =1 over water
$DX(h_x \text{ or } \delta_x)$	grid spacing (m)
$DY(h_y \text{ or } \delta_y)$	grid spacing (m)
EL (η)	the surface elevation as used in the external mode (m)
ET (η)	the surface elevation as used in the internal mode and derived from EL (m)
EG (η)	the surface elevation also used in the internal mode for the pressure gradient and derived from EL $(m)$
D (D)	= H + EL (m)
DT (D)	= H + ET (m)
DRX2D, DRY2D	vertical integrals of DRHOX and DRHOY
H (H)	the bottom depth (m)
SWRAD	short wave radiation incident on the ocean surface (m s <sup>-1</sup> K)
UA, VA, $\left(\overline{\operatorname{U}},\overline{\operatorname{V}}\right)$	vertical mean of U, V (m s <sup>-1</sup> )
UT, VT, $\left(\overline{\operatorname{U}},\overline{\operatorname{V}}\right)$	UA, VA time averaged over the interval, DT = DTI (m s <sup>-1</sup> )
WUSURF, WVSURF	$(\langle wu(0)\rangle, \langle wv(0)\rangle)$ momentum fluxes at the surface $(m^2s^{-2})$
WUBOT, WUBOT	( <wu(-1)>,<wv(-1)>) momentum fluxes at the bottom (m<sup>2</sup>s<sup>-2</sup>)</wv(-1)></wu(-1)>
WTSURF, WSSURF	$(<\!w\theta(0)\!>,<\!ws(0)\!>)$ temperature and salinity fluxes at the surface (ms $^{\text{-}1}$ K, ms $^{\text{-}1}$ psu)

#### Three-Dimensional Arrays

ADVX, ADVY horizontal advection and diffusion terms in equations (3-2) and (3-3)

AAM  $(A_M)$  horizontal kinematic viscosity  $(m^2 s^{-1})$ AAH  $(A_H)$  horizontal heat diffusivity = TPRNI\*AAM

CURV  $(\widetilde{f})$  curvature terms

 $L\left(\ell\right)$  turbulence length scale

KM  $(K_M)$  vertical kinematic viscosity  $(m^2 s^{-1})$ 

KH ( $K_H$ ) vertical diffusivity ( $m^2 s^{-1}$ )

DRHOX x-component of the internal baroclinic pressure gradient

$$\left( g D h_y \rho_0^{-1} \left[ -D \! \int_\sigma^0 \, \delta_x \rho' \delta \sigma' + \delta_x D \! \int_\sigma^0 \, \sigma' \delta \rho' \right] \right) \ \, \text{subtract RMEAN from density before integrating}$$

DRHOY *y*-component of the internal baroclinic pressure gradient

 $\left( g D h_x \rho_0^{-1} \bigg[ - D \! \int_\sigma^0 \, \delta_y \rho' \delta \sigma' + \delta_y D \! \int_\sigma^0 \, \sigma' \delta \rho' \bigg] \right)$  subtract RMEAN from density before integrating

RAD (R) short wave radiation flux (ms<sup>-1</sup>K). Sign is the same as WTSURF



Table 9-1.	Fortran Symbols	(Cont.)
------------	-----------------	---------

Indices	Description
Q2 (q <sup>2</sup> )	twice the turbulence kinetic energy (m <sup>2</sup> s <sup>-2</sup> )
QL $(q^2\ell)$	Q2 × the turbulence length scale (m³s⁻²)
T (T)	potential temperature (K)
S (S)	salinity (psu)
RHO ( $\rho/\rho_{o}$ -1.025)	density (non-dimensional)
U, V (U, V)	horizontal velocities (m s <sup>-1</sup> )
W (ω)	sigma coordinate vertical velocity (m s <sup>-1</sup> )
RMEAN	density field which is horizontally averaged before transfer to sigma coordinates.
TCLIM	a stationary temperature field which approximately has the same vertical structure as T.
SCLIM	a stationary salinity field which approximately has the same vertical structure as S.

#### 9.2 Program Structure

The ECOMSED computer programs consist of a main program and a set of subroutines. The main program and subroutines contain approximately 15,000 lines of code and they share a common file of some 100 or so records. The file "comdeck" must be edited for new values of IM, JM, KB or KSL (number of standard level). The various components of the computer programs are listed in Table 9-2. Figure 9-1 is the flow chart for the programs in simplified form. The code is written in a modular fashion so that various "physics" packages can be inserted easily. For example, SUBROUTINE PROFQ solves for the vertical mixing coefficients (eddy viscosity and eddy diffusivity). If forms other than the presently implemented level 2-1/2 turbulence closure model are desired, they can be incorporated in a new subroutine and PROFQ discarded. Much care has gone into the design of a code that is fully vectorizable. The use of "IF" statements has been greatly minimized. The code has a five fold increase in speed when running with vectorization "on" o n X - MP / 48a Crav supercomputer.



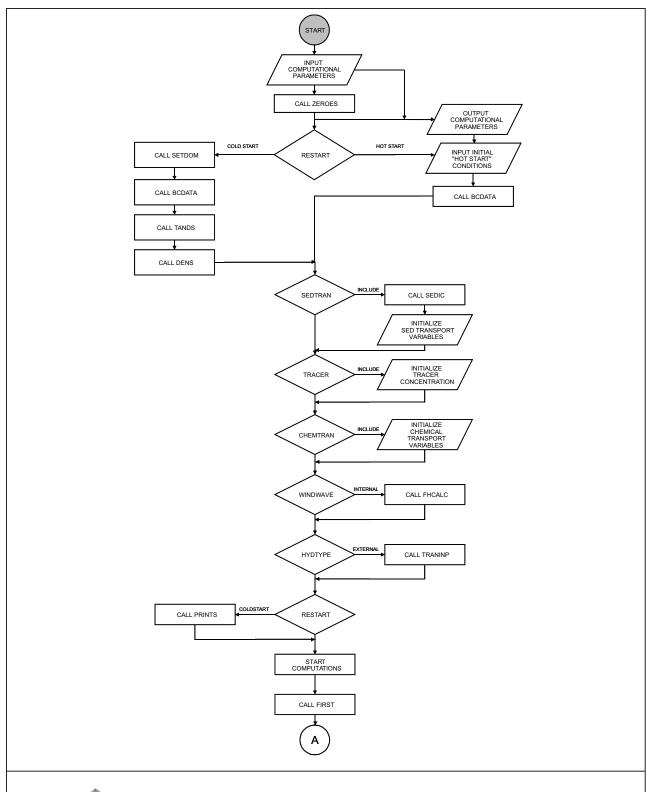
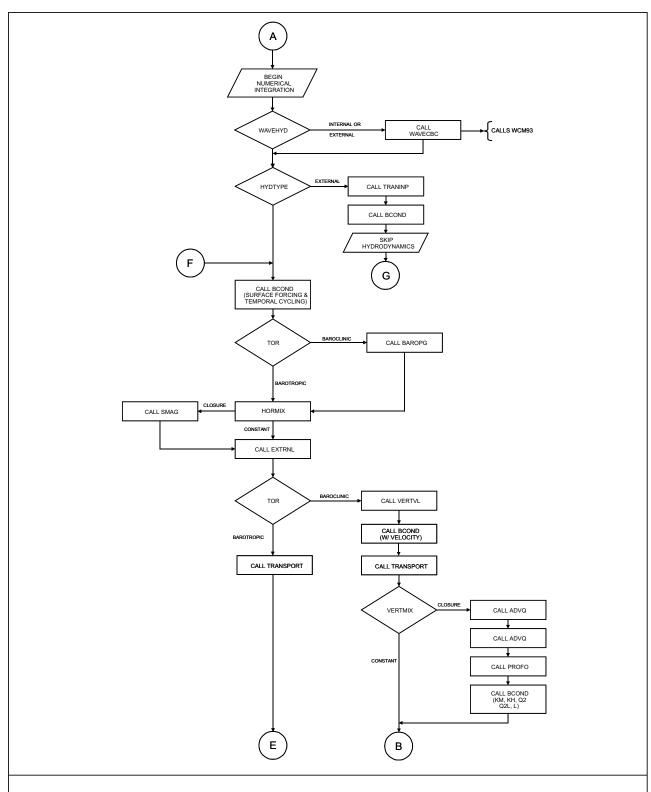
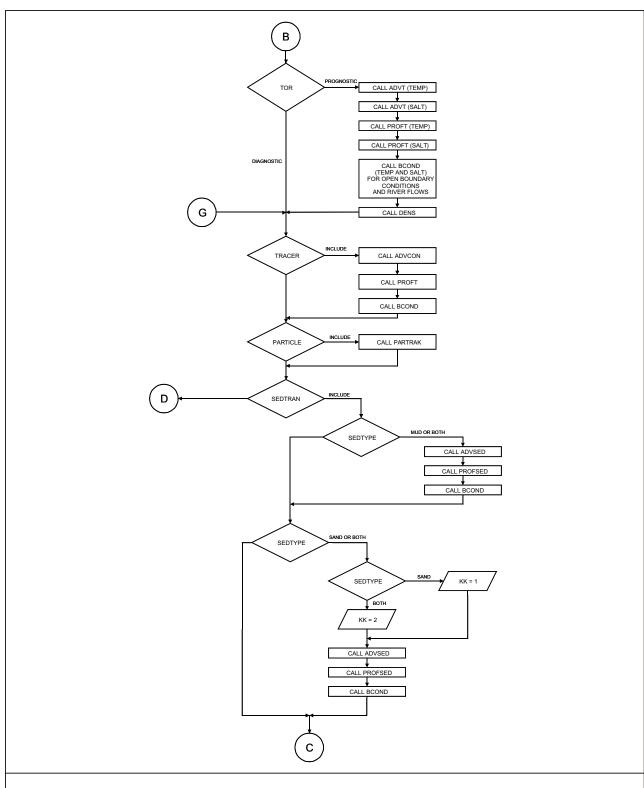




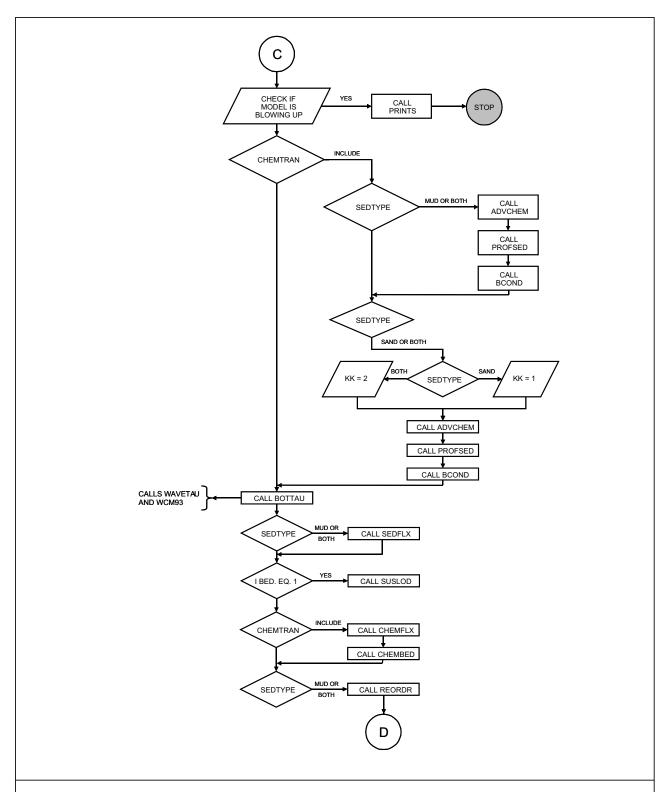
FIGURE 9-1













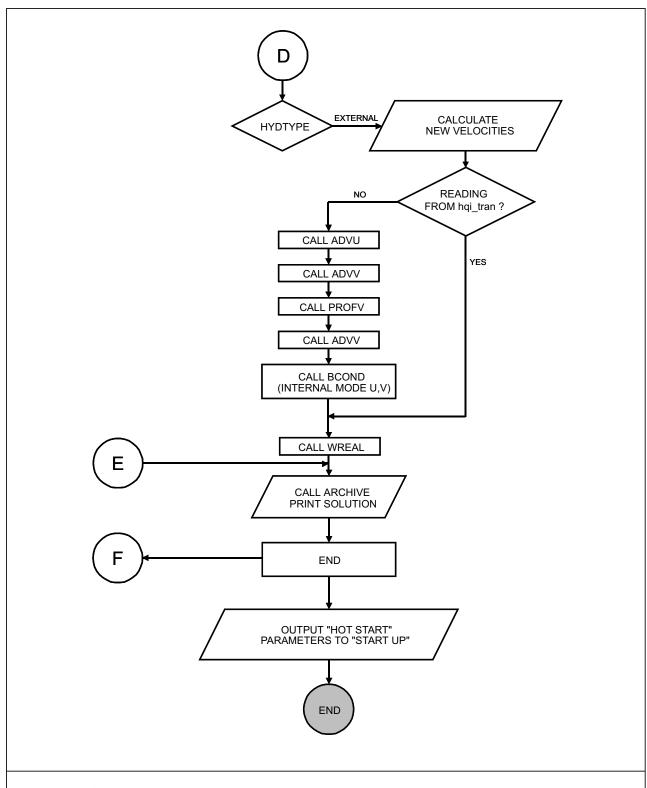




Table 9-2. Components of the Computer Programs

Subroutines	Description
ADVAVE	Computes the advective and dispersive terms in the $\xi_{\scriptscriptstyle 1}$ and $\xi_{\scriptscriptstyle 2}$ components of the vertically integrated momentum equation
ADVCHEM	Computes advective and dispersive terms in sediment-bound tracer transport equation
ADVCON	Computes advective and dispersive terms in dissolved tracer transport equation
ADVQ	Computes the advective and dispersive terms in the turbulence kinetic energy and macroscale equations
ADVSED	Computes advective and dispersive terms in sediment transport equation
ADVT	Computes the advective and dispersive terms in the mass transport equation
ADVU	Computes the advective, Coriolis, pressure gradient and dispersive terms in the $\xi_{\mbox{\tiny 1}}$ component of the momentum equation
ADVV	Computes the advective, Coriolis, pressure gradient and dispersive terms in the $\xi_{\!\scriptscriptstyle 2}$ component of the momentum equation
ANTIDIF	Computes anti-diffusion velocities for use in Smolarkiewicz transport algorithm
ARCHIVE	Time averages and writes to disk various quantities useful for graphical analyses
BAROPG	Computes the baroclinic pressure gradient terms through the vertical integral of the horizontal density gradient
BCDATA	Reads in the boundary condition data and performs the necessary interpolation for the model run
BCOND	Specifies the lateral and surface boundary conditions. Cycles through the input files when necessary
BOTTAU	Computes bottom shear stresses for sediment transport model
BULK	Computes sensible heat and latent heat
CHEMBED	Calculates changes in sediment bed concentrations of sediment-bound tracer
CHEMFLX	Calculates flux of sediment-bound tracer at sediment-water interface
COMDECK	Contains all paramters, type specifications, dimensions and common blocks to be included in the main program and subroutines. COMDECK should be edited for new values of IM, JM, KB and KSL.
DENS	Computes the local density of water from the most recent values of temperature and salinity. The program actually uses $\rho\text{-}1$
DISPLY	Writes a two dimensional array to the "gcmprt" file



Table 9-2. Components of the Computer Programs

Subroutines	Description
ECOM3D	Controls and monitors the flow of the particular simulation. This is the main program
EXTRNL	Solves for the depth integrated U and V velocities
FHCALC	Calculates fetch and mean depth for wind wave model
FIRST	Prepares the first set of data for use in the time variable model run
FZOL	Estimates stability functions for heat flux calculation
JDAY	Gives Julian day number
LONGWAVE	Computes longwave radiation
MAXMIN	Finds the maximum and minimum values of an array
N_CLOUD	Estimates total shortwave radiation reaching the earth surface and cloud cover fraction (0.0 to 1.0)
NCLD	Calculates percent cloud cover based on observed shortwave radiation and day of the year
ONEPART	Particle tracking algorithm
PARTRAK	Controls particle tracking simulations
PRINT	Writes a two dimensional array to the "gcmprt" file in an integer format
PRINTS	Controls the printing of the various model quantities
PROFE	Solves for empirical vertical mixing coefficients
PROFQ	Solves for turbulence kinetic energy, turbulence macroscale, and the vertical mixing coefficients for momentum, and temperature and salinity
PROFT	Solves for temperature, salinity and conservative tracer
PROFU	Solves for the U velocity
PROFV	Solves for the V velocity
PRTXY	Selects a horizontal field for use in PRINT
QSAT	Calculates saturation humidity
REORDR	Reorders sediment layers due to consolidation
SEDFLX	Calculates sediment flux at sediment-water interface
SEDIC	Initializes sediment transport constants and variables
SETDOM	Defines the physical characteristics of the model domain and the particular run and computes various constants to expedite the computation
SINTER	Interpolates various data profiles to model depths from their observed depth



Table 9-2. Components of the Computer Programs

Subroutines	Description
SLICEXZ	Writes a vertical slice in the x-direction of a three dimensional array to the "gcmprt" file
SLICEYZ	Writes a vertical slice in the y-direction of a three dimensional array to the "gcmprt" file
SMAG	Computes the coefficient of horizontal viscosity
STRESS	Calculates bottom shear stress due to wind induced waves and currents
SUSLOD	Calculates non-cohesive sediment suspended load
TANDS	Prepares the initial temperature and salinity fields for use in the model calculation
TRANINP	Reads external hydrodynamic information from "hqi_geom" and "hqi_tran" files
TRANSPORT	Calculates mean mass transport fields for use with a water quality model
VAPOR	Computes vapor pressure
VERTVL	Solves for the vertical velocity
WAVEDON	Calculates wave parameters based on Donelan (1977)
WAVESMB	Calculates wave parameters based on United States Army Corps of Engineers Shore Protection Manual (1984)
WREAL	Computes the vertical velocity in real x, y, z space
ZEROES	Sets all computational arrays to initial zeroes and values

The information necessary to make a complete ECOMSED model run is contained in 24 files, briefly described in Table 7.3. Also described briefly in Table 7-3 are the model generated output files and are followed by detailed descriptions of the contents of certain output files.



Table 9-3. Mass Storage Files

iab	Table 9-3. Mass Storage Files								
	User Created Files	Description							
1.	model_grid	Contains the physical information for the model grid (needed if $\mbox{HYDTYPE} = \mbox{"INTERNAL"})$							
2.	init_tands	Contains the initial conditions for temperature and salinity in each water grid box at the standard levels noted in run data (needed if HYDTYPE = "INTERNAL")							
3.	run_data	Contains parameters which control the type and length of the simulation. The frequency of various outputs is also included here, along with some of the important problem constants							
4.	synop_wind	Contains time variable wind components and atmospheric pressure for the entire model grid. This file is an unformatted input file							
5.	synop_hflx	Contains time variable surface heat flux data for the entire model grid. This file is an unformatted input file							
6.	corner_loc	Contains corner locations of grid elements, used for wind wave simulations when WAVEHYD = "INTERNAL" and needed for particle tracking simulations							
	NOTE	The following user created file is needed for dissolved tracer transport calculations (TRACER = "INCLUDE")							
7.	water_tracer.inp	Contains input parameters and boundary condition values for dissolved tracer transport.							
	NOTE	The following user created files are needed for sediment transport calculations (SEDTRAN = "INCLUDE")							
8.	coh_sed.inp	Contains input parameters and boundary condition values for cohesive sediment transport (needed if SEDTYPE = "MUD" or "BOTH")							
9.	noncoh_sed.inp	Contains input parameters and boundary condition values for non-cohesive sediment transport (needed if SEDTYPE = "SAND" or "BOTH"							
10.	bed_mask	Contains sediment bed map for the entire model grid							
11.	p0_init	Contains initial values of spatially-variable cohesive bed fractions for the entire model grid							
12.	a0_init	Contains spatially-variable $a_{\scriptscriptstyle 0}$ values for the entire model grid							
13.	exp_init	Contains spatially-variable values of exponent n for the entire model grid							
14.	bed_d50	Contains spatially-variable $D_{50}$ values for the entire model grid							
15.	bed_frac.mud	Contains spatially-variable cohesive composition fractions for the entire model grid, clay/silt fraction							
16.	bed_frac.sand	Contains spatially-variable cohesive composition fractions for the entire model grid, sand fraction							
17.	bed_bulkden	Contains spatially-variable sediment bed bulk density for the entire model grid							
	NOTE	The following user created files are needed for sediment-bound tracer transport calculations (CHEMTRAN = "INCLUDE" and SEDTRAN = "INCLUDE")							
18.	coh_trace.inp	Contains input parameters and boundary condition values for cohesive sediment-bound tracer transport (needed if SEDTYPE = "MUD " or "BOTH")							



Table 9-3. Mass Storage Files

User Created Files	Description
19. noncoh_trace.inp	Contains input parameters and boundary condition values for non-cohesive sediment-bound tracer transport (needed if SEDTYPE = "SAND" or "BOTH")
20. bed_chemic	Contains spatially-variable initial bed concentrations for sediment-bound tracer, for the entire model grid
NOTE:	The following user created file is needed for particle tracking calculations (PARTICLE = "INCLUDE")
21. partrack.inp	Contains input parameters for particle tracking
NOTE:	The following user created files are needed for simulations using externally-calculated hydrodynamics (HYDTYPE = "EXTERNAL")
22. hqi_geom	This file contains grid segmentation information to be used for transport calculations
23. hqi_tran	This file contains the computed results as a time history for surface elevations and hydrodynamic advection/dispersion fields to be used for transport calculations
NOTE	The following user created file is needed for simulations using externally-calculated wind wave fields (WAVEHYD = "EXTERNAL")
24. wave_input	This file contains computed results as a time history for wind wave parameters as calculated using a wind wave model (e.g., WAM or HISWA
Model Generated Files	Description
1. gcmprt:	This file is a main output file containing all the input information and all the computed values
2. gcmplt	This file contains the computed results as a time history for all grid elements. It is useful for graphical analyses
3. gcmtsr	This file contains the computed values of elevation, current, temperature and salinity, and cross sectional fluxes for user specified grid elements. This file also contains the run-time global integrals of various parameters to assist in the diagnosis of the model
4. gcm_tran	This file contains the computed results as a time history for surface elevations, volume transports and dispersions to be used by a water quality model
5. gcm_geom	This file contains grid segmentation information to be used by a water quality model
6. startup	This file contains all the information for the hydrodynamic model run which will become the initial conditions for the "HOT START" runs
7. restart	This file is similar to the "startup" file. User should move or copy the "startup" file to "restart" before making the next "HOT START" run



# 10.0 Model Input Data Structure

This section provides a detail description of data structure of 24 input data files and selected output files. The names of the input/output files are listed in Section 7.

# 10.1 Model Geometry Input Data

The input file name is model\_grid. There are three data groups in this input file (Table 10-1A).

Table 10-1A: model\_grid data structure

Data Group	Description
A.	Comment for Grid Information
B.	Vertical Segmentation
	Comment
	Number of sigma levels
	Sigma levels
C.	Horizontal Segmentation
	Comment
	I index and J index
	Grid Information

NOTE: The model\_grid file is only needed if HYDTYPE = "INTERNAL".

Table 10-1B describes in detail format of the data structure in model\_grid.



Table 10-1B: model\_grid data format

<u>Data Group A</u>: Comment for Grid Information

COM = user specified comment for grid information

<u>Data Group B</u>: Vertical Segmentation

1. <u>Comment</u>

COM = user specified comment for sigma levels

2. <u>Number of Sigma Levels</u>

IKB = number of sigma levels

3. <u>Sigma Levels</u>

Z = depth of the interface between sigma levels

 $-1.0 \le Z \le 0.0$ 

 $\underline{NOTE}$ : Total number = IKB.



Data Group C: Horizontal Segmentation

#### 1. Comment

COM user specified comment for horizontal segmentation

#### 2. I Index and J Index

index in the  $\xi_1$  direction index in the  $\xi_2$  direction IIX IJY

#### Grid Information 3.

**XGRID** 

5	1 0	20	30	40	50	60	70	75	80
ı	J	H1	H2	Н	ANG	YGRID	XGRID	DATUM	

2I5,4F10.2,2F10.5,F5.1,I5

Ι I number of grid element in the  $\xi_1$  direction j number of grid element in the  $\xi_2$  direction J H1 distance in meters in the  $\xi_1$  direction at center of grid element distance in meters in the  $\xi_2$  direction at center of grid element H2 Н = average depth of grid element in meters (at mean water level) MLW + tidal amplitude

**ANG** angle in degrees between east and  $\xi_1$  direction measured in a counter-clockwise direction

**YGRID** = latitude of grid center in degrees (positive for northern hemisphere) to compute

the Coriolis parameter longitude of grid center in degrees (Note: model does not use this. Only used

for postprocessing purposes)

DATUM =datum of grid element in meters (above some reference elevation)

## NOTE:

Total number of wet grid ≤ total number of grid elements. Grid information need be specified for wet points only and it is not necessary to specify grid information for other grid elements. H must be sufficiently large in order to remain wet at low tide.



<u>Data Group D</u>: Specification of Thin Dams

1. <u>Comment</u>

COM = user specified comment for thin dams.

2. Number of Thin Dams

NOTE: If there is no thin dam specified in the model domain, user can either specify NUMTDAM = 0 or skip Data Group D.

2. <u>Location of Thin Dams</u>

ISTDAM(N) = I number of grid element in which thin dam begins JSTDAM(N) = j number of grid element in which thin dam begins

DIRTDAM(N) = direction of thin dam (cross-section)

"IDIR" - cross-section is in the  $\xi_1$  direction "JDIR" - cross-section is in the  $\xi_2$  direction

NTDAM(N) = number of grid elements in the thin dam cross-section



## 10.2 Initial Condition

The initial condition input file name is "init\_tands". There is only one data group. Tables 8-2A and 8-2B describe the data structure and format respectively.

Table 10-2A: Data structure of init\_tands

Data Group	Description
A.	Location, Temperature and Salinity at Standard Levels
NOTE:	The init_tands file is only needed if HYDTYPE = "INTERNAL"

Table 10-2B: init\_tands data format

Data Group A: Location, Temperature and Salinity at Standard Levels

5	10	15		20		260	265	270		510
1	J	TS(I,J,1)		TS (I,J,2)		TS(I,J,KSL)	SS(I,J,1)	SS(I,J,2)		SS(I,J,KSL)
215,	100F5.0									
I = I number of grid element in the $\xi_1$ direction J = j number of grid element in the $\xi_2$ direction TS = temperature in °C at each standard level SS = salinity in psu at each standard level										
NOTE:  1. KSL = number of standard levels. To ensure proper interpolation of da standard level to sigma level, each bottom-most sigma level must be br by two standard levels. These standard levels must contain data.								st be bracketed		



# 10.3 Model Simulation Input Data

The name of the input file is run\_data. This file contains parameters which control the type and length of the simulation. The frequency of various output is included here. The data also contains various modeling contents. There are eight data groups as listed in Tables 8-3A and 8-3B.

Table 10-3A. Data structure of run\_data

	Data Structure of run_uata							
Data Group	Description							
A.	Run Computational, Output and Print Characteristics Comment Comment-Run options Run options Comment-Run computational characteristics Run computational characteristics Comment-Run output characteristics Run output characteristics Comment-Run print characteristics Run print characteristics							
В.	Hydrodynamic Characteristics Comment-Constants of the model problem Constants of the model problem Comment-Horizontal mixing characteristics Horizontal mixing characteristics Comment-Vertical mixing characteristics Vertical mixing characteristics							
C.	Result Evaluation Computational history for plotting Comment Number and averaging interval of computational history output sets Time in number of time steps for writing the output Averaging interval for skill assessment Comment Averaging interval Computed time series for elevations Comment Number of grid elements Location of grid elements Computed time series for currents, temperature, salinity & transport quantities Comment Number of grid elements Comment Number of grid elements Computed time series for cross sectional fluxes Comment Number of cross sections Location of cross sections Location of cross sections Computational results for water quality							



# Table 10-3A. Data structure of run\_data

Data Group	Description								
	Comment								
	Number and averaging interval of computational result output sets								
	Time in number of time steps for writing the output								
D.	Standard Level Declaration								
	Comment								
	Number of standard levels								
	Standard levels								
E.	Initial Temperature and Salinity Data								
	Comment								
	Initial temperature and salinity data option								
	Initial temperature data								
	Initial salinity data								
F.	Open Boundary Condition Information								
	Elevation boundary conditions								
	Comment								
	Number of grid elements and option								
O 11 4	Elevation boundary conditions								
Option 1	Time variable data								
	Location of grid elements								
	Time of observation								
Ontion 0	Elevation data								
Option 2	Computer generated data from tidal constituents  Location of grid elements and mean water level								
	Amplitudes of the 6 dominant harmonic constituents								
	Phases of the 6 dominant harmonic constituents								
	Time Variable temperature and salinity boundary conditions								
	Comment								
	Temperature and salinity boundary conditions								
	Time of observation								
	Location of grid elements, temperature and salinity data								
G.	Discharge Information								
	Time variable river/dam and onshore intake/outfall discharges								
	Comment								
	Number of grid elements								
	Location of grid elements/vertical distribution of intake/outfall								
	discharge								
	Time of observation								
	Discharge data								
	Temperature data								
	Salinity data								
	Time variable offshore intake/outfall (diffuser) discharges								
	Comment								
	Number of grid elements								
	Location of grid elements/vertical distribution of intake/outfall diffuser discharge								



## Table 10-3A. Data structure of run\_data

Data Group	Description
	Time of observation
	Discharge data
	Temperature data
	Salinity data
	Time variable offshore intake/outfall (diffuser) discharges in loops
	Comment
	Number of grid elements
	Location of grid elements/vertical distribution of intake/outfall diffuser discharge
	Time of observation
	Discharge data
	Temperature data
	Time variable offshore intake/outfall discharges in loops
	Comment
	Grid elements (I,J) and distribution of flows
	Discharge data
	Temperature data
	Salinity data
H.	Meteorological Data
	Comment
	Meteorological data option
0 11 4	Meteorological data
Option 1	Time variable surface heat data, salt flux data and wind data
	Time of observation
Ontine 0	Precipitation, evaporation, heat flux, wind speed and direction data
Option 2	Synoptic time variable surface heat flux data and synoptic wind and atmospheric pressure data
	Wind and pressure data input from file "synop_wind"
	Surface heat flux data input from file "synop_hflx"
Option 3	Time variable surface heat flux parameters, salt flux data and wind data
	Time of observation
	Precipitation, evaporation, heat flux, wind speed and direction data



Table 10-3B: Data format of run\_data

## **DATA GROUP A:** Computational and Output Characteristics

1. <u>Comment</u>

80 COM 80A1

COM = user specified comment for run information

2. Comment - Run Options

80 COM 80A1

COM = user specified header for run options

3. Run Options

10203040506070HYDTYPEWAVEDYNTRACERSEDTRANCHEMTRANSEDTYPEPARTICLE

2X,A8,2X,A8,3X,A7,3X,A7,3X,A7,6X,A4,3X,A7

HYDTYPE = "INTERNAL" - use internal (ECOM) hydrodynamics

= "EXTERNAL" - use external hydrodynamics input from 'hqi\_tran' file

WAVEDYN = "NEGLECT" - no effect of surface waves on bottom friction

= "SMBMODEL" - include effects of waves on bottom friction, internal

calculation of waves using SMB theory

= "DONMODEL" - include effects of waves on bottom friction, internal

calculation of waves using Donelan Theory

= "EXTERNAL" - include effects of waves on bottom friction, wave parameters input from 'wave\_input' file, (external calculation using WAM

or HISWA)

TRACER = "INCLUDE" - dissolved tracer transport will be simulated

"NEGLECT" - no simulation of dissolved tracer transport

SEDTRAN = "INCLUDE" - sediment transport will be simulated

"NEGLECT" - no simulation of sediment transport

CHEMTRAN = "INCLUDE" - sediment-bound tracer transport will be simulated

"NEGLECT" - no simulation of sediment-bound transport



SEDTYPE = "BOTH" - cohesive and non-cohesive sediment transport

"MUD" - cohesive sediment transport only

= "SAND" - non-cohesive sediment transport only

PARTICLE = "INCLUDE" - particle tracking will be simulated

= "NEGLECT" - no simulation of particle tracking

NOTE: SMBMODEL is not fully operational.

<u>NOTE</u>: CHEMTRAN = "INCLUDE" requires that SEDTRAN = "INCLUDE".

NOTE: CHEMTRAN option is not fully operational.

## 4. Comment - Run Computational Characteristics

25

COM = user specified header to identify run computational characteristics

35 40

45

## 5. Run Computational Characteristics

DTI	ISPLIT	IRAMP	IYR	IMO	IDA	IHR	NHYD	SGW	WETEPS	WETMIN	TUNIT
A10,I5,	A10,I5,F5.0,5I5,F5.0,2F10.0,A5										
DTI		=							`	imum allov .RI (user sp	
ISPL	IТ	=	time s	teps to er of ti	be uso me sto	ed in ' eps be	ʻtimestep etween th	.inp" fil e intern	e)	ernal mode	
NOT IRAN		=	If TO	refer to Section 8.1 for more details.  If TOR = "PROGNOSTIC" or "DIAGNOSTIC", ISPLIT >3 number of time steps over which all model forcing functions are ramped							
,	IMO, , IHR	=					lues linea of model	,	ne and IYI	R should b	e a 4-digit
NHY		=	numbe	er er of ti	me ste	eps be	tween ea	ch hydr	odynamic	transport f	
SGW	7	=	semi-p Please	rogno see	stic co Section	efficie n 8-4	nt based of for de	on Shen tails.	If SGW	ERNAL" .tch and Wa = 1 and stic mode (	TOR =
WET	TEPS	=	1.0) water conne	elevati ction f	on dif	ferenc	ces betwe	een dry cell (u	cell and w	vet cell to when CS, then the	determine the water

cell will be flooded. Recommended value: 0.1 m or higher.

= minimum water elevation retained in the drying cell (unit: meter).



WETMIN

Recommended value: 0.3 m or higher.

TUNIT

= time unit for NSTEPS, IRAMP, IPRINT, IPRTSTART. TUNIT can be "DAY", " ", or "NDTI", if no option is specified, model assumes "NDTI" as TUNIT

## 6. Comment - Run Output Characteristics

COM = user specified header to identify NSTEPS, IPRINT, IPRTSTART, RESTAR, TOR, ADVECT output characteristics

# 7. Run Output Characteristics

IPRINT	IPRT	START	RESTART	TOR	ADVECT	SCHEME	SEDRESTART	
),1X,A10,1X	,A10,	1X,A10,1X	(,A8					
20	_	مدم طب	mation angail	End in '	CHNITT IF	TUNIT	"DAV" NOTEDC:	
33	_			11eu 111 .	IUNII. II	TUNIT 18	DAI , NOTEPOIS	rum
Τ	=	print in	nterval in nu	mber o	f time steps	3		
TART	=						vill begin	
١R	=							
	=							
	=							l in
						`		
	=		,	- 3-D c	alculation (	bottom str	ess calculated in PRO	FU
					`			
	=		,	- 3-D	calculation	with temp	erature and salinity h	neld
						1	,	
	=		P-ONLY" -	3-D pr	ognostic ru	n while init	ial salinity values are h	neld
	=					while initi	al temperature fields	are
						- ,,	v	
СТ	=					on terms		
	=						on terms	
ME	=							
	=							
	=							ing
								/ <del></del> 8
	=						Smolarkiewicz and us	ino
								/ <del></del> 8
		· · · · · · · ·	0000 101 0011			car arragio	••	
ESTART	=	"COLI	DSEDS" - s	edimen	t bed initial	lized usino	the "core_field.sdf" f	ile
	=							the
	O,1X,A10,1X, PS T TART AR CT ME	D,1X,A10,1X,A10, PS = T = TART = TART = = = = = = = = =  CT = = = = = = = = = = = = = = = = = = =	PS = run duration T = print ir TART = time in AR = "COLI = "HOT = "BARC ADVA = "PROC & PROC = "DIAC fixed = "TEM throug = SALT- held th CT = "LINE = "NON ME = "CEN" = "SMON reclusive = "SMON two pa	PS = run duration specific duration in days  T = print interval in nu TART = time in number of of of order  R = "COLD START" - a = "BAROTROPIC" ADVAVE)  = "PROGNOSTIC" & PROFV)  = "DIAGNOSTIC" fixed  = "TEMP-ONLY" - order throughout the sim = SALT-ONLY" - order HOT START" - a = "BAROTROPIC" ADVAVE)  = "PROGNOSTIC" fixed  = "TEMP-ONLY" - order Horoughout the sim = SALT-ONLY" - order   "NON-LINEAR" - no m = "NON-LINEAR"  ME = "CENTRAL" - cer = "UPWIND" - upw = "SMOLAR_R" - fireclusive formulati = "SMOLAR_2" - fireclusive form	PS = run duration specified in a duration in days  T = print interval in number of time state  TART = time in number of time state  TART = "COLD START" - all initial  = "HOT START" - all initial  = "BAROTROPIC" - 2-1  ADVAVE)  = "PROGNOSTIC" - 3-D of the state  **PROFV**  = "DIAGNOSTIC" - 3-D produced throughout the simulation  = SALT-ONLY" - 3-D produced throughout the simulation  = SALT-ONLY" - and produced throughout the simulation  = "LINEAR" - no momentum of the same of the sa	PS = run duration specified in TUNIT. If duration in days  T = print interval in number of time steps at which the steps at whi	PS = run duration specified in TUNIT. If TUNIT is duration in days  T = print interval in number of time steps  TART = time in number of time steps at which printing varieties are set to the steps at the printing varieties are set to the steps at the printing varieties are set to the steps at the printing varieties are set to the step at the printing varieties are set to the step at the printing varieties are set to the step at the printing varieties are set to the step at the printing varieties are set to the step at the printing varieties are set to the step at the printing varieties are set to the step at the printing varieties are set to the step at the printing varieties are set to the step at the st	PS = run duration specified in TUNIT. If TUNIT is "DAY", NSTEPS is duration in days  T = print interval in number of time steps  TART = time in number of time steps at which printing will begin  RR = "COLD START" - all initial conditions are set to zero  = "HOT START" - all initial conditions are input from file "restart"  = "BAROTROPIC" - 2-D calculation (bottom stress calculated aDVAVE)  = "PROGNOSTIC" - 3-D calculation (bottom stress calculated in PRO & PROFV)  = "DIAGNOSTIC" - 3-D calculation with temperature and salinity fixed  = "TEMP-ONLY" - 3-D prognostic run while initial salinity values are fully throughout the simulation  = SALT-ONLY" - 3-D prognostic run while initial temperature fields held throughout the simulation  CT = "LINEAR" - no momentum advection terms  = "NON-LINEAR" - include momentum advection terms  ME = "CENTRAL" - central finite difference scheme for advection  = "UPWIND" - upwind finite difference scheme for advection  = "SMOLAR_R" - finite difference scheme due to Smolarkiewicz and us reclusive formulation for antidiffusive velocities  = "SMOLAR_2" - finite difference scheme due to Smolarkiewicz and us two passes for corrections of numerical diffusion



"SEDRESTARTFILE" file.

<u>NOTE</u>: If RESTAR = "HOT START", then the user should move or copy "startup"

to "restart" before the model run. "startup" is a file containing computed

results from the previous model run.

If TOR = "BAROTROPIC", ISPLIT = 1

If TOR = "PROGNOSTIC" or "DIAGNOSTIC", ISPLIT >3

NOTE: HOT START option is not fully operational for Particle Tracking and wave

simulations.

#### 8. Comment - Run Print Characteristics

80 COM 80A1

COM = user specified header to identify run print characteristics of variables DEV, VSX, JROW, VSY, IROW, U, V, W, AM, S, T, RHO, Q2, L, KM, KH for output to "gcmprt"and netCDF output

### 9. Run Print Characteristics

5	10	15	20	25	30	35	40
DEV	VSX	JROW	VSY	ICOL	U	٧	W
45	50	55	60	65	70	75	80
	- 00		- 00		, ,	, 0	- 00
AM	S	Т	RHO	Q2	L	KM	KH

2X,A3,4X,A1,I5,4X,A1,I5,11(4X,A1)

DEV = primary output device for viewing "gcmprt"

= "SCR" - for 15 columns across the page, suitable for printing on a screen

with no wrap around

= "LPR" - for 25 columns across the page, suitable for printing on a laser

or line printer

VSX = vertical slice in the x  $(\xi_1)$  direction of various model quantities included in

the "gcmprt" file

= "Y" - vertical slices

= "N" - no vertical slices

JROW = j number at which the vertical slice in the x  $(\xi_1)$  direction will be taken

= 0, for VSX="N"

VSY = vertical slice in the y  $(\xi_2)$  direction of various model quantities included in



4	Λ	Λ
ı	v	٠u

		the "gcmprt" file
	=	"Y" - vertical slices
	=	"N" - no vertical slices
ICOL	=	I number at which the vertical slice in the y ( $\xi_2$ ) direction will be taken
	=	0, for VSY="N"
U	=	U velocity included in "gcmprt"
	=	"Y" - include
	=	"N" - omit
V	=	V velocity included in "gcmprt"
	=	"Y" - include
	=	"N" - omit
W	=	W velocity included in "gcmprt"
	=	"Y" - include
	=	"N" - omit
AM	=	horizontal mixing included in "gcmprt"
	=	"Y" - include
	=	"N" - omit
S	=	salinity and conservative tracer included in "gcmprt"
	=	"Y" - include
	=	"N" - omit
Τ	=	temperature included in "gcmprt"
	=	"Y" - include
	=	"N" - omit
RHO	=	density included in "gcmprt"
	=	"Y" - include
	=	"N" - omit
Q2	=	turbulent kinetic energy included in "gcmprt" for closure vertical mixing
	=	"Y" - include
	=	"N" - omit
L	=	mixing length included in "gcmprt" for closure vertical mixing
	=	"Y" - include
****	=	"N" - omit
KM	=	mixing K <sub>M</sub> included in "gcmprt" for closure vertical mixing
	=	"Y" - include
1711	=	"N" - omit
KH	=	mixing K <sub>H</sub> included in "gcmprt" for closure vertical mixing
	=	"Y" - include
	=	"N" - omit



## **DATA GROUP B:** Hydrodynamic Characteristics

#### 1. <u>Comment - Constants of the Model Problem</u>

80 COM 80A1

COM = user specified header for BFRIC, ZOB, NU, ALPHA, TLAG constants

## 2. <u>Constants of the Model Problem</u>

10	20	30	40	50	60	70	80
BFRIC	ZOB	NU	THETA	ALPHA	TLAG	NWAVE	BCTYPE
6E10.2  10	1 2v 17						

6E10.3, I10, 3x,A7

BFRIC = minimum bottom friction coefficient (non-dimensional)

If user wants to specify spatially variable (2D) bottom friction coefficients, specify BFRIC as "VARI" (6X, A4) and provide "bfric2d.inp" file. Please refer to Table 10-26 for more details of format specification of "bfric2d.inp" file.

ZOB = bottom roughness coefficient in meters

NU = coefficient in time filter (non-dimensional)

0.1 (recommended value)

THETA = weighting factor (0-1); 0 - explicit and 1- implicit scheme

= 0.225 (recommended value)

ALPHA = advection time scale for temperature and salinity at the boundary time

"HOURS" over which the boundary values reach their full specified value during the flood cycle from the values exiting at the end of the ebb cycle. \*Caution: If the user does not want boundary relaxation ( $\alpha$ -folding), specify

ALPHA = 0.

TLAG = friction time scale (Hours) for barotropic radiation boundary condition (only

needed if user selects BCTYPE as PCLAMP

NWAVE = number of time steps between each update of bottom friction coefficient, only

used if WAVEHYD is not "NEGLECT"

BCTYPE = baratropic radiation boundary condition types

"CLAMPED" - clamp boundary condition (no radiation)

"PCLAMP" - partially clamped. Note: if user selects PCLAMP type B.C., user

must provide TLAG in Hours

"OCLAMP" - optimized clamp which is same as RANDB except  $\lambda t$  is non

unity.

"RANDB" - Reid and Bodine type boundary condition

"IRANDB" - inverted Reid and Bodine type boundary condition )( $\lambda_{\tau}$  = 1)



#### 3. Comment - Horizontal Mixing Characteristics

COM user specified header for HORZMIX, HORCON, HPRNU mixing characteristics

#### 4. Horizontal Mixing Characteristics

10	20	30
HORZMIX	HORCON	HPRNU
A10.2E10.3		

**HORZMIX** "CONSTANT" - value given for HORCON is scaled in each grid element

relative to the smallest grid element

"CLOSURE" - value given for HORCON is used in Smagorinsky's

formula for mixing

**HORCON** value used as a constant or in Smagorinsky's formula based on HORZMIX

(non-dimensional)

If user wants to specify spatially variable (2D) HORCON, specify HORCON as "VARI" (6X,A4) and provide "horcon2d.inp" file. Please refer to Table 10-25 for more details of format specification of "horcon2d.inp" file.

**HPRNU** horizontal Prandtl number - ratio of horizontal viscosity to

horizontal diffusivity (momentum mixing/dispersive mixing)

1.0 (recommended value)

#### 5. Comment - Vertical Mixing Characteristics

80 COM 80A1

COM user specified header for VERTMIX, UMOL, VPRNU mixing characteristics

#### Vertical Mixing Characteristics 6.

 10	20	30	40
VERTMIX	UMOL	VPRNU	BETA

A10,3E10.3 or A10,6X,A4,2E10.3 if umol is spatially variable

**VERTMIX** "CONSTANT" - value given for UMOL applies everywhere

"CLOSURE" - value given to UMOL is background mixing

"EMPIRICAL" - empirical vertical turbulent mixing based on Kent and



Pritchard (1959) and Offcer (1976)

UMOL = constant or background mixing in m²/sec
= 1.0E-06 (recommended value if VERTMIX = "CLOSURE") or "EMPIRICAL".

If user wants to specify spatially variable (2D) UMOL, specify UMOL as

If user wants to specify spatially variable (2D) UMOL, specify UMOL as "VARI" (6X.A4) and provide "umol2d.inp" file. Please refer to table 10-27 for more details of format specification of "umol2d.inp" file

VPRNU = vertical Prandtl number - ratio of vertical viscosity to vertical diffusivity (momentum mixing/diffusive mixing) for VERTMIX = "CONSTANT"

= If VERTMIX = "EMPIRICAL", VPRNU acts as coefficient  $\alpha$  in the

empirical mixing equation (8-9a) = Coefficient  $\beta$  in the empirical mixing equation (8-8 and 8-9) if VERTMIX

= "EMPIRICAL". For other VERTMIX options, BETA will be ignored.

= 1.0 (recommended value)

## DATA GROUP C: Result Evaluation

**BETA** 

### 1. <u>Computational History Output for Plotting</u>

#### a. Comment

COM = user specified comment for computational history output

b. Number and Averaging Interval of Computational History Output Sets

10	20	30	40	45	50
JHM	AVGE	IPLTFORM	PLTZERO	OPTAVG	OUTFORM
		= •		0	001101111

I10, F10.3, 65X,A4, F10.2, 1X, A4,2X,A3

JHM = number of times all information necessary for plotting will be written in

"gcmplt" and "part\_location" (if PARTICLE = "INCLUDE")

AVGE = interval in number of time steps or hours for averaging the elevations,

temperature, salinity and currents for all grid elements

IPLTFORM = "USER" or "(left in blank spaces") user specifies the "gcmplt" output

intervals.

"AUTO" output interval will be generated by ECOMSED based on the

values of PLTZERO, AVGE and JHM

PLTZERO = The beginning timestep or hour of "gcmplt" output (TZERO)

OPTAVG = indicating the units of AVGE and PLTZERO. "HOUR": time control is

in hour,

"NDTI": time control is in number of timesteps.

If the OPTAVG is in hour and AVGE is not an integer multiple of timestep ECOMSED will stop and ask for another AVGE period.



OUTFORM = Output format of "gcmplt" file.

"BIN": Binary output format "CDF": netCDF output format

If OUTFORM = "CDF", please refer to Data Group A.9 for the selection

of output parameters.

<u>NOTE</u>: If JHM = 0 or IPLTFORM = "AUTO", then go to Data Group C.2 (Averaging Interval for Skill Assessment)

c. <u>Time in Number of Time Steps for Writing the Output</u>

IHIST = time in number of time steps all information will be written in "gcmplt" and "part\_location" (for particle tracking output when PARTICLE =

"INCLUDE")

NOTE: IHIST relative to start of run (independent of RESTART option specified)

## 2. Averaging Interval for Skill Assessment

a. Comment

COM = user specified comment for averaging interval for skill assessment

b. Averaging Interval

ISKILL = interval in number of time steps for averaging the elevations, temperature, salinity and currents and cross sectional fluxes for user

specified grid elements (for example, at the tide gauge locations)

= 0, no element stored in "gcmtsr" for skill assessment

NOTE: If ISKILL=0, then go to Data Group C.6 (Computational Results for Water

Quality Model)



- 3. <u>Computed Time Series for Elevations</u>
  - a. <u>Comment</u>

COM = user specified comment for computed time series for elevations

b. <u>Number of Grid Elements</u>

EPTS = number of grid elements for which time series of elevations are to be stored in "gcmtsr"

NOTE: If EPTS=0, then go to Data Group C.4 (Computed Time Series for Currents, Temperature and Salinity)

c. <u>Location of Grid Elements</u>

INXIE = I number of grid element INXIE = j number of grid element

- 4. Computed Time Series for Currents, Temperature, Salinity and Transport Quantities
  - a. <u>Comment</u>

COM = user specified comment for computed time series for temperature, salinity and currents

b. <u>Number of Grid Elements</u>



VPTS = number of grid elements for which time series of temperature, salinity

and currents are to be stored in "gcmtsr"

NOTE: If VPTS=0, then go to Data Group C.5 (Computed Time Series for Cross

Sectional Fluxes)

c. <u>Location of Grid Elements</u>

5	10	 75	80
INXIV(1)	INXJV(1)	 INXIV(VPTS)	INXJV(VPTS)
16l5			

INXIV = I number of grid element INXIV = j number of grid element

5. <u>Computed Time Series for Cross Sectional Fluxes</u>

a. Comment

COM = user specified comment for computed time series for cross sectional fluxes

b. Number of Cross Sections

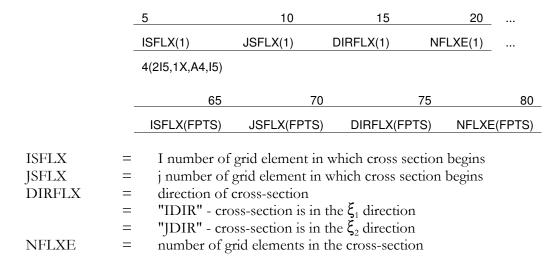
FPTS = number of cross sections for which time series of fluxes are to be stored

in "gcmtsr"

NOTE: If FPTS=0, then go to Data Group C.6 (Computation Results for Water

Quality Model)

### c. Location of Cross Sections



### 6. <u>Computation Results for Water Quality Model</u>

#### a. <u>Comment</u>

80 COM 80A1

COM = user specified comment for computation results for water quality model

## b. Number and Averaging Interval of Computation Result Output Sets

10	20	30	40	50
JTM	NPLPF	ITRNFORM	IZERO	IWET
5110				

JTM = number of times all information necessary for the water quality model

input is generated

NPLPF = interval in number of time steps for averaging the elevations and currents

to be used as input in the water quality model

ITRNFORM = 0: user specified time steps for writing the output

1: ECOM will generate the writing block (i.e. section 6.c.)

IZERO = # of time steps to skip before start to writing 'gcm\_tran' information.

IZERO should not be '0' if 'COLD START'. If ITRNFORM = 0,

IZERO will be ignored.

IWET = 0: entire grid output

1: wet grid only output



## 10.0 Model Input Data Structure

NOTE: If JTM = 0, then go to Data Group D (Standard Level Declaration)

c. <u>Time in Number of Time Steps for Writing the Output</u>

IF ITRANFORM = 0

IF ITRANFORM = 1 skip this block

8	16	 80
ITRAC(1)	ITRAC(2)	 ITRAC(JTM)
1018		

**ITRAC** 

time in number of time steps at which the information will be output, necessary for water quality model input

NOTE:

ITRAC relative to start of run (independent of RESTART option specified)

## **DATA GROUP D:** Standard Level Declaration

1. <u>Comment</u>

COM = user specified comment about the standard levels

2. Number of Standard Levels

IKSL = number of standard levels (< 50)

<u>NOTE</u>: To reduce the amount of computer storage required, keep the number of standard levels (IKSL) at a minimum, i.e., IKSL < 50.

### 3. Standard Levels

	10	20	 80
	DPTHSL(1)	DPTHSL(2)	 DPTHSL(IKSL)
8	3F10.5		

DPTHSL = depth of standard level in meters with respect to surface water level

NOTE:

It is not necessary to include the surface level, although it may be included. If not, constituent values associated with the first level below the surface will be applied to the depth between the surface and the first standard level. Extrapolation to the surface may cause incorrect representation of the vertical profile. To ensure proper interpolation of data from standard level to sigma level, each bottom-most sigma level must be bracketed by two standard levels. These standard levels must contain data.

## **DATA GROUP E**: Initial Temperature and Salinity

### 1. Comment

COM = user specified comment for temperature and salinity data

## 2. <u>Initial Temperature and Salinity Data Option</u>

**OPTTSI** 

= "FIXED" - initial temperature and salinity data are constant for each standard level.

= "DATA" - initial temperature and salinity data vary horizontally and vertically - data read in from data file "init\_tands".

If OPTTSI = "DATA", then go to Data Group F (Open Boundary Condition Information)

#### 3. <u>Initial Temperature Data</u>



4. <u>Initial Salinity Data</u>

## **DATA GROUP F:** Open Boundary Condition Information

## 1. <u>Elevation Boundary Conditions</u>

a. Comment

b. Number of Grid Elements and Option

5	26
NUMEBC	OPTEBC
I5,1X,A20	

NUMEBC = total number of elevation boundary grid elements. If NUMEBC = 0,

then go to Data Group G (Discharge Information)

OPTEBC = "DATA" - use Elevation Boundary Conditions OPTION 1 - Time

Variable Data

= "TIDAL CONSTITUENT" - use Elevation Boundary Conditions

OPTION 2 - Computer Generated Data from Tidal Constituents

c. <u>Elevation Boundary Conditions</u>

## **OPTION 1 - TIME VARIABLE DATA**

I. Location of Grid Elements



5	10	15	20	
IETA(1)	JETA(1)	ICON(1)	JCON(1)	
16l5				

65	70	75	80
IETA(NUMEBC)	JETA(NUMEBC)	ICON(NUMEBC)	JCON(NUMEBC)

IETA = I number of grid element where elevation is specified JETA = j number of grid element where elevation is specified

ICON = I number of connecting grid element (nearest interior non-boundary grid

element)

JCON = j number of connecting grid element (nearest interior non-boundary grid

element)

NOTE: Every boundary element should have a connecting interior grid element.

#### ii. Time of Observation

10 TIME F10.5

TIME = time in hours

= 0.0 for initial time

NOTE: TIME is absolute time measured from beginning of COLD START run and

incremented with each subsequent HOT START run.

## iii. Elevation Data

 10
 20
 30
 ...
 80

 EBDRY(1)
 EBDRY(2)
 EBDRY(3)
 ...
 EBDRY(NUMEBC)

 8F10.5

EBDRY = boundary elevation data in meters at time "TIME"

<u>NOTE</u>: Sequence (TIME/EBDRY) repeated for each observation. Final "TIME" must

be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT

START runs.



#### **OPTION 2 - COMPUTER GENERATED DATA FROM TIDAL CONSTITUENTS**

#### I. Location of Grid Elements and Mean Water Level

		5	10	15	20	30	
		IETA	JETA	ICON	JCON	EMEAN	
		4I5,F10.5					
IETA	=	I number o	of grid elem	ent			
JETA	=	j number o	of grid eleme	ent			
ICON	=	I number o	of connecting	g grid elem	ent (neares	t interior nor	n- boundary grid
		element)					, ,
JCON	=	j number o	f connecting	grid eleme	ent (neares	t interior nor	n- boundary grid
3		element)			`		, 0
<b>EMEAN</b>	=	mean wate	r level in me	eters with re	eference to	the lowest r	nean water level
		of entire de	omain				

### ii. Amplitudes of the 6 Dominant Harmonic Constituents

 10	20	30	40	50	60
AMP-S <sub>2</sub>	AMP-M <sub>2</sub>	AMP-N <sub>2</sub>	AMP-K₁	AMP-P₁	AMP-O₁

6F10.5

AMP-S<sub>2</sub> solar semidiurnal amplitude in meters (period = 12.00 hr) AMP-M<sub>2</sub> lunar semidiurnal amplitude in meters (period = 12.42 hr) = $AMP-N_2$ = lunar semidiurnal amplitude in meters (period = 12.66 hr) lunar diurnal declination amplitude in meters (period = 23.94 hr) AMP-K<sub>1</sub> = = solar diurnal declination amplitude in meters (period = 24.06 hr) AMP-P<sub>1</sub> lunar diurnal declination amplitude in meters (period = 25.82 hr)  $AMP-O_1$ 

#### iii. Phases of the 6 Dominant Harmonic Constituents

10	20	30	40	50	60
PHASE-S <sub>2</sub>	PHASE-M <sub>2</sub>	PHASE-N <sub>2</sub>	PHASE-K₁	PHASE-P₁	PHASE-O₁
6F10.5					

PHASE-S<sub>2</sub> = solar semidiurnal phase in degrees (period = 12.00 hr)

PHASE-M<sub>2</sub> = lunar semidiurnal phase in degrees (period = 12.42 hr)

PHASE-N<sub>2</sub> = lunar semidiurnal phase in degrees (period = 12.66 hr)

PHASE-K<sub>1</sub> = lunar diurnal declination phase in degrees (period = 23.94 hr)

PHASE-P<sub>1</sub> = solar diurnal declination phase in degrees (period = 24.06 hr)

PHASE-O<sub>1</sub> = lunar diurnal declination phase in degrees (period = 25.82 hr)

NOTE:

Every boundary element should have a connecting interior grid element. Sequence i/ii/iii repeated for each boundary element. Total number = NUMEBC (total number of elevation boundary grid elements). Phases of each component are in degrees and are with respect to Greenwich Mean Time.



## 2. <u>Time Variable Temperature and Salinity Boundary Conditions</u>

a. Comment

COM = user specified comment for temperature and salinity boundary conditions

- b. Temperature and Salinity Boundary Conditions
  - i. Time of Observation

TIME = time in hours

= 0.0 for initial time

NOTE: TIME is absolute time measured from beginning of COLD START run and incremented with each subsequent HOT START run.

ii. Location of Grid Elements, Temperature and Salinity Data

	5			1	10						15							20	)	
ΓΑ	S			JTA	S	TBE	DRYS	SL(N	UMI	EBC	;,1)		TE	DRY	SL(	NUI	ИΕΕ	3C,2	)	
0	F5.0																			
					260						26	5						270	1	
_	2)// /\			<u> </u>					/h II				0.5		·01 /		455			•••
TBDRSYL(NUMEBC,IKSL)					S	BDF	(YSL	J(NL	JIVIE	BC,	1)	SE	DRY	SL(	NUI	/IEE	3C,2	)		

ITAS = i number of grid element where temperature and salinity are specified JTAS = j number of grid element where temperature and salinity are specified

TBDRYSL = temperature in °C at time "TIME" for each standard level (not sigma

level)

SBDRYSL = salinity in psu at time "TIME" for each standard level (not sigma level)

1. Sequence (ITAS/JTAS/TBDRYSL/SBDRYSL) repeated for each location. Total number = NUMEBC (total number of boundary grid elements). The sequence (TIME/ TBDRYSL/SBDRYSL) repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater

than IEND + (NSTEPS x DTI)/3600 for HOT START runs. TIME for



NOTE:

- temperature and salinity observation need not be the same as for elevation observations.
- 2. The ITAS, JTAS sequence of temperature/salinity boundary conditions must correspond exactly to the IETA, JETA sequence of elevation boundary conditions, i.e., ITAS = IETA and JTAS = JETA for n=1 to n=NUMEBC.



## **DATA GROUP G:** Discharge Information

# 1. <u>Time Variable River/Dam and Onshore Intake/Outfall Discharges</u>

a. <u>Comment</u>

80 COM 80A1

COM = user specified comment for discharge

b. Number of Grid Elements

NUMQBC

location.

NUMQBC

total number of discharge boundary grid elements. If NUMQBC = 0, then go to Data Group G.2 (Time Variable Offshore Intake/Outfall (Diffuser) Discharges)

Sequence (IQD/JQD/IQC/JQC/VQDIST) is repeated for each discharge

15

20

c. <u>Location of Grid Elements/Vertical Distribution of Intake/Outfall Discharge</u>

5

	<u>-</u>	IQD(NUMQBC) 4I5,20F5.0	JQD(NUMQBC)	IQC(NUMQBC)	JQC(	NUMQBC)
	=	25	30	35_		120
	=	VQDIST(1)	VQDIST(2)	VQDIST(3)		VQDIST(KBM1)
IQD JQD IQC JQC VQDIST	= = =	j number of gr i number of co	apporti	rge enters/leaver boundary grid e boundary grid e age (not fraction) oned to each mo	s lement lement of tota del laye	al discharge QDIS er from surface to
KBMI	=	KB-1	bottom	at location (IQI	),JQD)	

10



NOTE:

### d. Time of Observation

10 TIME F10.5

TIME = time in hours

= 0.0 for initial time

NOTE: TIME is absolute time measured from beginning of COLD START run and

incremented with each subsequent HOT START run.

### e. Discharge Data

10	20	30	 80
QDIS(1)	QDIS(2)	QDIS(3)	 QDIS(NUMQBC)
8F10.5			

**QDIS** 

= discharge flow in m<sup>3</sup>/sec

> 0.0 (positive) for flow into the model domain (river/outfall)

< 0.0 (negative) for flow out of the model domain (intake)

## f. <u>Temperature Data</u>

10	20	30	 80
TDIS(1)	TDIS(2)	TDIS(3)	 TDIS(NUMQBC)
8F10.5			

TDIS = temperature of discharge in °C

#### g. Salinity Data

10	20	30	 80
SDIS(1)	SDIS(2)	SDIS(3)	 SDIS(NUMQBC)
8F10.5			

SDIS = salinity of discharge in psu

NOTE:

Sequence (TIME/QDIS/TDIS/SDIS) repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs. Discharges leaving the model domain (intakes) do not require associated T and S values. However, a value of zero should be input as



the values for T and S of these discharges.

# 2. <u>Time Variable Offshore Intake/Outfall (Diffuser) Discharges</u>

a. Comment

COM = user specified comment for discharge

b. Number of Grid Elements

NUMDBC 1 = total number of discharge grid elements. If NUMDBC = 0, then go to Data Group G3 (Time Variable Offshore Intake/Outfall (Diffuser) Discharges in Loops)

c. <u>Location of Grid Elements/Vertical Distribution of Intake/Outfall Diffuser Discharge</u>

5	10	15	20	 110
IDD(NUMDBC)	JDD(NUMDBC)	VDDIST(1)	VDDIST(2)	 VDIST(KBM1)
2I5,20F5.0				

IDD = i number of grid element diffuser enters/leaves

JDD = j number of grid element diffuser enters/leaves

VDDIST = percentage (not fraction) of total discharge DQDIFF apportioned each

model layer from surface to bottom at location (IDD, JDD)

KBM1 = KB-1

NOTE: 1. Sequence (IDD/JDD/VDDIST) is repeated for each diffuser location.

2. More than one diffuser can be specified at the same location (IDD, JDD)

d. Time of Observation



TIME = time in hours

= 0.0 for initial time

NOTE:

TIME is absolute time measured from beginning of COLD START run and incremented with each subsequent HOT START run.

e. <u>Discharge Data</u>

QDIFF = diffuser discharge in m<sup>3</sup>/sec

f. Temperature Data

TDIFF = temperature of diffuser discharge in °C

g. Salinity Data

SDIFF = salinity of diffuser discharge in psu

NOTE:

Sequence (TIME/QDIFF/TDIFF/SDIFF) repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs. Discharges leaving the model domain do not require associated T and S values. However, a value of zero should be input as the values for T and S of these discharges.

## 3. <u>Time Variable Offshore Intake/Outfall (Diffuser) Discharges in Loops</u>

a. Comment

COM = user specified comment for discharge in loops



5 NUMDBC2

NUMDBC2

total number of discharge grid elements. If NUMDBC2 = 0, then go to Data Group H (Meteorological Data). The NUMDBC2 should be even numbers; intake/outfall diffusers are specified in pairs; diffuser is intake and the other is recirculating discharging outfall (i.e., one diffuser discharges the volume of water withdrawn through the other)

c. <u>Location of Grid Elements/Vertical Distribution of Intake/Outfall Diffuser Discharge</u>

5	10	15	20	 110
IDD(NUMDBC)	JDD(NUMDBC)	VDDIST(1)	VDDIST(2)	 VDIST(KBM1)
2I5,20F5.0				

IDD = i number of grid element diffuser enters/leaves JDD = j number of grid element diffuser enters/leaves

VDDIST = percentage (not fraction) of total discharge DQDIFF apportioned each

model layer from surface to bottom at location (IDD,JDD)

KBM1 = KB-1

NOTE:

Sequence (IDD/JDD/VDDIST) is repeated for each intake/outfall diffuser location.

## d. Time of Observation

TIME = time in hours

= 0.0 for initial time

NOTE: TIME is absolute time measured from beginning of COLD START run

and incremented with each subsequent HOT START run.

## e. <u>Discharge Data</u>

10	20	 80
DQDIFF(1)	DQDIFF(2)	 DQDIFF(NUMDBC2)
8F10.5		



**DQDIFF** 

= diffuser discharge in m³/sec. Even though DQDIFF(N) and DQDIFF(N+1) is a coupling intake/outfall pair, the DQDIFF(N) and DQDIFF(N+1) need not be equal.

# f. Temperature Data

10	20	30	 80
DTDIFF(1)	DTDIFF(2)	DTDIFF(3)	 DTDIFF(NUMDBC2)
8F10.5			

**DTDIFF** 

= temperature increase/decrease of diffuser discharge in °C. Only effective on diffuser having positive values of DQDIFF. This increase/decrease of temperature is with respect to the temperature of corresponding intake.

### g. Salinity Data

10	20	30	 80
DSDIFF(1)	DSDIFF(2)	DSDIFF(3)	 DSDIFF(NUMDBC2)
8F10.5			

**DSDIFF** 

= salinity increase/decrease of diffuser discharge in psu. Only effective on diffuser having positive values of DQDIFF.

NOTE:

Sequence (TIME/DQDIFF/DTDIFF/DSDIFF) repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs. Discharges leaving the model domain do not require associated T and S values. However, a value of zero should be input as the values for T and S of these discharges.



# **DATA GROUP H:** Meteorological Data

### 1. <u>Comment</u>

80 COM 80A1

COM = user specified comment for meteorological data

# 2. <u>Meteorological Data Option</u>

10	20	30	40	50	60	70
OPTMBC	ALAT	ALON	TR	WNDSH	REFL	OPTEXTC

A10,5F10.2, 6X,A4

OPTMBC = "AVERAGED" - a single value for each meteorological parameter is used for all grid element at each time - use Meteorological Data OPTION 1 - Time Variable Surface Heat Flux Data, Salt Flux Data and Wind Data

- = "SYNOPTIC" spatially varying meteorological parameter values are specified for every grid element at each time use Meteorological Data OPTION 2 Averaged Time Variable Surface Heat Flux Data and Salt Flux Data and Synoptic Time Variable Wind and Atmospheric Pressure Data
- = "AANDBFLX" heat flux sub-model based on the work of Ahsan and Blumberg (1999). The local heat flux is determined from local surface temperature use Meteorological Data OPTION 3 Time Variable Surface Heat Flux Parameters, Salt Flux Data and Wind Data
- = "LANDPFLX" heat flux sub-model based on the work of Large and Pond (1982). The local heat flux is determined from local surface temperature use Meteorological Data OPTION 3 Time Variable Surface Heat Flux Parameters, Salt Flux Data and Wind Data.
- = "RANDMFLX" heat flux sub-model based on the work of Rosati and Miyakoda (1988). The local heat flux is determined from local surface temperature use Meteorological Data OPTION 3 Time Variable Surface Heat Flux Parameters, Salt Flux Data and Wind Data.
- = "SYNOPANB", "SYNOPLNP", "SYNOPRNM": These options allow the user to specify spatially varying wind data along with heat flux sub-model options "AANDBFLX", "LANDPFLX", and "RANDBFLX", respectively.

ALAT = Latitude (in degrees, median of modeling domain)

ALON = Longitude (in degrees, median of modeling domain) (0  $\sim$  -180 for western

hemisphere)

TR = Fraction of short wave radiation absorbed in surface layer

WNDSH = Wind sheltering coefficient (default = 1.0)

REFL = Reflection of shortwave radiation at surface (0.0-1.0) (0.0 - nothing



reflected; 1.0 - complete reflection) 0.1 (recommended value)

OPTEXTC = Option for extinction coefficients. If "VARI", spatially varying extraction

coefficients specified in "extc2d.inp" will be used. If OPTEXTC is left in blank or other than "VARI", the model will use time-varying but spatially

uniform EXTC specified in OPTION 3 below.

# 3. Meteorological Data

#### OPTION 1 - Time Variable Surface Heat Flux Data, Salt Flux Data and Wind Data

### i. <u>Time of Observation</u>

10 TIME F10.5

TIME = time in hours

= 0.0 for initial time

NOTE: TIME is absolute time measured from beginning of COLD START run and

incremented with each subsequent HOT START run.

# ii. Precipitation, Evaporation, Heat Flux, Wind Speed and Direction Data

		10	20	30	40	40	
		WDS	WDD	HFLUX	QPREC	QEVAP	_
WDS	=	5F10.5 wind speed	d in m/sec	:			

WDD = direction of wind in degrees from which the wind blows, measured

clockwise from north

 $HFLUX = heat flux in watts/m^2$ 

> 0, heating of the water

< 0, cooling of the water

QPREC = amount of precipitation in m/year QEVAP = amount of evaporation in m/year

NOTE: Sequence (TIME/QPREC/QEVAP/HFLUX/ WDS/WDD) repeated for each

observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than (IEND +

NSTEPS) x DTI/3600 for HOT START runs.



# OPTION 2 - Synoptic Time Variable Surface Heat Flux Data, Synoptic Wind, and Atmospheric Pressure Data

i. Wind and atmospheric pressure data input from file "synop\_wind" (Table 8-4A)

ii Surface Heat Flux Data Input from File "synop\_hflx" (Table 8-4B)

#### OPTION 3 - Time Variable Surface Heat Flux Parameters, Salt Flux Data and Wind Data

# i. <u>Time of Observation</u>

TIME = time in hours

= 0.0 for initial time

NOTE: TIME is absolute time measured from beginning of COLD START run and

incremented with each subsequent HOT START run.

# ii Precipitation, Evaporation, Heat Flux, Wind Speed and Direction Data

10	20	30	40	50
WDS	WDD	SWOBS	AIRTMP	RELHUM
60	70	80	90	100
BAROP	CLD	EXTC	QPREC	QEVAP

10F10.5

WDS = wind speed in m/sec

WDD = direction of wind in degrees from which the wind blows, measured

clockwise from north

SWOBS = observed shortwave radiation in watts/ $m^2$ 

AIRTMP = air temperature in °C

RELHUM = relative humidity in percent BAROP = barometric pressure in mbar CLD = cloud cover fraction (0.0 to 1.0)

EXTC = extinction coefficient

QPREC = amount of precipitation in m/year QEVAP = amount of evaporation in m/year



NOTE:

S e q u e n c e (T I M E / Q P R E C / Q E V A P / A I R T M P / RELHUM/BAROP/SWOBS/WDS/WDD) repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run) for COLD START runs, and greater than (IEND + NSTPS) x DTI/3600 for HOT START runs.



Table 10-4A. synop\_wind INPUT FILE SUMMARY OF DATA GROUPS

Data Group	Description
A.	Time Variable Synoptic Wind and Atmospheric Pressure Data
	Time of observation
	Wind and atmospheric pressure data

synop\_wind INPUT FILE (UNFORMATTED)

# Data Group A

1. <u>Time</u>

**TIME** 

TIME = time of observation

= 0.0 for initial time

<u>NOTE</u>: TIME is absolute time measured from beginning of COLD START run

and incremented with each subsequent HOT START run.

2. Wind and Atmospheric Pressure Data

//TY2D/L I) TY2D/L I) DATM/L I) L 1 IM) L 1 IM)

((TX2D(I,J),TY2D(I,J),PATM(I,J),I=1,IM),J=1,JM)

TX2D = velocity component in m/sec in the east-west direction TY2D = velocity component in m/sec in the north-south direction

PATM = atmospheric pressure in mb

NOTE: Sequence (TIME/TX2D/TY2D) repeated for each observation. Final

"TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS

x DTI)/3600 for HOT START runs.



Table 10-4B. synop\_hflx INPUT FILE SUMMARY OF DATA GROUPS

Data Groups	Description
A.	Time Variable Synoptic Surface Heat Flux Data
	Time of observation Surface heat flux data

synop\_hflx INPUT FILE (UNFORMATTED)

# Data Group A

1. Time

**TIME** 

TIME = time of observation

= 0.0 for initial time

NOTE: TIME is absolute time measured from beginning of COLD START run

and incremented with each subsequent HOT START run.

# 2. Surface Heat Flux Data

 $\substack{((SHFLX(I,J),I=1,IM),J=1,\\JM)}$ 

SHFLX = surface heat flux in  $w/m^2$ 

NOTE: Sequence (TIME/SHFLX) repeated for each observation. Final

"TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS

x DTI)/3600 for HOT START runs.



# Table 10-5. corner\_loc INPUT FILE

Table 8-5 lists the format of corner\_loc that contains corner locations of grid elements for wind, wave and particle tracking simulations. For transport calculations, user created input files are summarized in Table 8-6. Tables 8-7 through 8-24 list the detailed formats of those files. Model generated output files are summarized in Table 8-25. Tables 8-26 through 8-30 list the detailed format of some selected model output files in Table 8-25.

NOTE: PARTICLE = "INCLUDE" 5 10 30 XCOR(I,J) YCOR(I,J) 2I5, 2F10.0 i number of corner location in  $\zeta_1$  direction Ι j number of corner location in  $\zeta_2$  direction XCOR(I,J)corner location in x-direction (East), in meters YCOR(I,J)corner location in y-direction (North), in meters NOTE: Notation convention is XCOR(I,J) = x(i-1/2, j-1/2) and YCOR(I,J) = y(i-1/2, j-1/2)j-1/2) (Lower left hand corner of element)



Table 10-6. Summary of User Created Input Files for Transport Calculations

File	Description
water_tracer.inp	Contains input parameters and boundary condition values for dissolved
water_tracer.inp	tracer transport.
coh_sed.inp	Contains input parameters and boundary condition values for cohesive sediment transport.
noncoh_sed.inp	Contains input parameters and boundary condition values for non-cohesive sediment transport.
coh_trace.inp	Contains input parameters and boundary condition values for cohesive sediment-bound tracer transport.
noncoh_trace.inp	Contains input parameters and boundary condition values for non-cohesive sediment-bound tracer transport.
partrack.inp	Contains input parameters for particle tracking.
bed_mask	Contains sediment bed map for the entire model grid.
p0_init	Contains spatially-variable, initial cohesive bed fractions for the entire model grid.
a0_init	Contains spatially-variable $\mathbf{a}_0$ values for the entire model grid.
exp_init	Contains spatially-variable values of exponent n for the entire model grid.
bed_d50	Contains spatially-variable $D_{50}$ values for the entire model grid.
bed_frac.mud	Contains spatially-variable cohesive composition fractions for the entire model grid, clay/silt fraction.
bed_frac.sand	Contains spatially-variable cohesive composition fractions for the entire model grid, sand fraction.
bed_bulkden:	Contains spatially-variable sediment bed bulk density for the entire model grid.
bed_chemic:	Contains spatially-variable initial bed concentrations for sediment-bound tracer for the entire model grid.
NOTE:	All of the above input files are formatted.
hqi_geom:	Contains grid segmentation information to be used for transport calculations.
hqi_tran:	Contains the computed results as a time history for surface elevations and hydrodynamic advection/dispersion fields to be used for transport calculations.
wave_input:	Contains computed results as a time history for wind wave parameters as calculated using a wind wave model (e.g., WAM or HISWA).
NOTE:	These three files are unformatted.



## Table 10-7. water\_trace.inp INPUT FILE

<u>NOTE</u>: This file must be included for dissolved tracer transport simulations. (TRACER = "INCLUDE")

# 1. <u>Comment - Dissolved Tracer Input Parameters</u>

80 COM 80A1

COM = user specified comment for dissolved tracer input parameters

### 2. <u>Dissolved Tracer Input Parameters</u>

10	20	30	40	50	60	70	80
TROPT	TRICOPT	CONDRAT	CONINIT	THETAT	VSRATE	ASOL	ASAL
A10,5X,A	5,6F10.3						

TROPT = "CONSERV" - Conservative tracer (CONDRAT = 0.0)
"SIMPDECAY" - simple first order decay. Non-zero value of CONDRAT is required.

"PATHOGEN" - pathogen fate simulation. If TROPT = "PATHOGEN", user should specify proper values for CONDRAT, CONINT, THETAT, VSRATE, ASOL, and ASAL.

TRICOPT = Initial condition of dissolved tracer option: "DATA" or "FIXED"

If TRICOPT = "DATA", user must provide "init\_tracer" file. Please refer to Table 10-28 for more details of format specification.

If TRICOPT = "FIXED", uniform value of CONINIT will be used.

CONDRAT = dissolved tracer decay rate (first-order decay) in

day-1

CONINIT = initial dissolved tracer concentration in mg/l, assumed spatially constant

THETAT = Temperature coefficient  $\theta$  (default - 1.07)

VSRATE = Settling rates of bacteria (m/day)

ASOL = Coefficient of insolation ( $\alpha$ )  $\alpha=1$ . If  $\alpha=0$  then no dependency of decay

on solar radiation

ASAL = Switch for decay rate dependency on salinity. ASAL = 1, salinity

dependent and ASAL = 0, no salinity dependency.

NOTE: To simulate tracer as conservative substances users have to assign CONDRAT

= 0, VSRATE = 0, ASOL = 0 and ASAL = 0.



3. Comment - Dissolved Tracer Concentrations at Open Boundaries

COM = user specified comment for dissolved tracer concentrations at open boundaries

4. Number of Grid Elements

NUMEBCTR = total number of open boundary elements at which dissolved tracer concentrations will be specified

5. <u>Time of Observation</u>

TIME = time in hours = 0.0 for initial time

6. Location of Grid Elements and Dissolved Tracer Data

5	10	15	20	25	
ITRED	JTRED	ITREC	JTREC	CBDRYSL1(1)	CBDRYSL1(IKSL)
4I5,100F5.	0				

ITRED = i number of grid element where dissolved tracer is specified JTRED = j number of grid element where dissolved tracer is specified

ITREC = i number of connecting grid element (nearest interior non-boundary grid

element)

JTREC = j number of connecting grid element (nearest interior non-boundary grid

element)

CBDRYSL1 = dissolved tracer concentration in mg/l at "TIME" for each standard level

(not sigma level)

NOTE: 1. Sequence (ITRED/JTRED/CBDRYSL1) is repeated for each location.

Total number = NUMEBCTR (total number of boundary grid elements). The sequence (TIME/CBDRYSL1) is repeated for each observation.



Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs. "TIME" for dissolved tracer observations need not be the same as for elevation observations in run\_data.

- If HYDTYPE = 'INTERNAL', then NUMEBCTR = NUMEBC (as specified in Data Group F, Table 8-3B: Open Boundary Condition Information in run\_data).
- If HYDTYPE = 'EXTERNAL', then dissolved tracer concentrations must be specified at all open boundaries in the domain.
- 7. Comment - Dissolved Tracer Concentrations at River Discharges

80 COM 80A1

COM user specified comment for dissolved tracer concentrations at river discharges

8. Number of Grid Elements

location.

total number of river discharges at which dissolved tracer concentrations NUMQBCTR =will be specified

9. Location of Grid Elements

	5 10 15 20
	ITRQD JTRQD ITRQC JTRQC
	415
ITRQD	= i number of grid element discharge enters
JTRQD	= j number of grid element discharge enters
ITRQC	= i number of connecting exterior boundary grid element
JTRQC	= j number of connecting exterior boundary grid element
NOTE:	Sequence ITRQD/JTRQD/ITRQC/JTRQC is repeated for each discharge



#### 10. Time of Observation

10 TIME F10.1

TIME = time in hours

= 0.0 for initial time

#### 11. Dissolved Tracer Data

10	20	30	80_
CDIS1(1)	CDIS1(2)	CDIS1(3)	CDIS1(NUMQBCTR)
8F10.1			

CDIS1 = dissolved tracer concentration of river discharge in mg/l

NOTE:

- 1. The sequence (TIME/CDIS1) is repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs. Discharges leaving the mode domain (shore-based intakes) do not require associated CDIS1 values. However, a value of zero should be input for CDIS1 of these discharges.
- 2. If HYDTYPE = 'INTERNAL', then NUMQBCTR = NUMQBC (as specified in Data Group G, Table 8-3B: Discharge Information in run\_data).
- 3. If HYDTYPE = 'EXTERNAL', then dissolved tracer concentrations **must** be specified at all river discharges in the domain.

NOTE:

Only include the next data group (items 12-14) if offshore discharges (diffuser outfalls) are specified in run\_data (NUMDBC > 0 in Data Group G (Table 8-3B): Discharge Information)

#### 12. Comment - Dissolved Tracer Concentrations at Offshore Discharges

80 COM 80A1

COM = user specified comment for dissolved tracer concentrations at offshore discharges

# 13. Number of Grid Elements

NUMDBCTR1 = total number of offshore discharges at which dissolved tracer concentrations will be specified

# 14. <u>Location of Grid Elements</u>

ITRDD = i number of grid element discharge enters JTRDD = j number of grid element discharge enters

NOTE: Sequence ITRDD/JTRDD is repeated for each discharge location

# 15. <u>Time of Observation</u>

TIME = time in hours = 0.0 for initial time

#### 16. Dissolved Tracer Data

10	20	30	80
CDIFF1(1)	CDIFF1(2)	CDIFF1(3)	
			CDIFF1(NUMDBCTR1)
8F10.1			-

CDIFF1 = dissolved tracer concentration of offshore discharge in mg/l

NOTE: The sequence (TIME/CDIFF1) is repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs.

# 17. Comment-Dissolved Tracer Concentrations at Offshore Discharges in Loops

COM

= user specified comment for dissolved tracer concentrations at offshore discharges in loops

#### 18. Number of Grid Elements

NUMDBCTR2 =

total number of offshore discharges in loops at which dissolved tracer concentrations will be specified

# 19. <u>Time of Observations</u>

TIME

= time in hours

= 0.0 for initial time

# 20. <u>Dissolved Tracer Data</u>

10	20	30	80
DCDIFF1(1)	DCDIFF1(2)	DCDIFF1(3)	DCDIFF1(NUMDBCTR2)
8F10.1			

DCDIFF1 = dissolved tracer concentrations of offshore discharge in loops in mg/l

NOTE:

The sequence (TIME/DCDIFF1) is repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLDSTART runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOTSTART runs.



# 21. Comment - Dissolved Tracer Point Source Loads

80 COM 80A1

COM = user specified comment for dissolved tracer point source loads

# 22. Number of Grid Elements and Point Source Loading Option

5 15 NUMPSTR OPTPSTR 15,6X,A4

NUMPSTR = total number of grid elements at which dissolved tracer point source loads

will be specified

OPTPSTR = "MASS" - dissolved tracer point sources are specified as a mass loading

in kg/s

= "CONC" - dissolved tracer point sources are specified as instantaneous concentrations in mg/l

### 23. <u>Location of Grid Elements</u>

5 10 15

IPSTR JPSTR KPSTR

315

IPSTR = i number of grid element where dissolved tracer point source is specified

JPSTR = j number of grid element where dissolved tracer point source is specified

KPSTR = k number of grid element where dissolved tracer point source is specified

NOTE: Sequence IPSTR/JPSTR/KPSTR is repeated for each point source location.

#### 24. <u>Time of Observation</u>

10 TIME F10.1

TIME = time in hours = 0.0 for initial time



# 25. Dissolved Tracer Data

10	20	80
PSLOAD(1)	PSLOAD(2)	PSLOAD(NUMPSTR)
8F10.1		

PSLOAD = dissolved tracer load in kg/s (OPTPSTR = "MASS")

= dissolved tracer load in mg/l (OPTPSTR = "CONC")

NOTE:

- 1. If OPTPSTR = "CONC", then the point source load is specified by instantaneously setting the dissolved tracer concentration in grid element (IPSTR, JPSTR, KPSTR) equal to PSLOAD (mg/l) at the specified time whenever PSLOAD > 0. No point source load will be specified at all times that PSLOAD = 0 mg/l.
- 2. The sequence (TIME/PSLOAD) is repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run) for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs.

NOTE:

"TIME" for all the above boundary conditions is absolute time measured from beginning of COLD START run and incremented with each subsequent HOT START run.



## Table 10-8. coh\_sed.inp INPUT FILE for SEDZL

<u>NOTE</u>: This file must be included for cohesive sediment transport simulations.

(SEDTRAN = "INCLUDE" and SEDTYPE = "BOTH" or "MUD")

1. <u>Comment - Sediment Transport Control Parameters</u>

COM = user specified comment for sediment transport control parameters

2. Sediment Transport Control Parameters

NSEDBEG = time step at which to start sediment transport calculation

NSBED = frequency, in time steps, at which to calculate deposition/ resuspension

fluxes

NOTE: If SEDTYPE = "BOTH", then NSEDBEG and NSBED must have the same

values in both coh\_sed.inp and noncoh\_sed.inp.

3. <u>Comment - Cohesive Sediment Deposition Parameters</u>

COM = user specified comment for cohesive sediment deposition parameters

4. <u>Cohesive Sediment Deposition Parameters</u>

 10	20	30	40
 ADEP	DEPEXP	TCRDEP	PDEPFORM

3F10.0, 5X,A5

ADEP =  $A_{set}$  coefficient for floc settling speeds in  $\mu$ m/s

DEPEXP = b exponent for floc settling speeds

TCRDEP = critical shear stress for deposition of cohesive sediment in dynes/cm<sup>2</sup> PDEPFORM = "KRONE" - Krone formulation for probability of deposition (TCRDEP

 $= \tau_d \text{ in Eq. 5-11}$ 



"PARTH" - Partheniades formulation for probability of deposition (TCRDEP =  $\tau_{b,min}$  in Eq. 5-13)

5. <u>Comment - Cohesive Sediment Resuspension Parameters</u>

80 COM 80A1

COM = user specified comment for cohesive sediment resuspension parameters

6. Cohesive Sediment Resuspension Parameters

 10
 20
 30
 40

 A0IN
 RESEXP
 EXPM
 VARIAON

 3F10.0, 3X,A7

A0IN =  $a_0$  parameter in Eq. (5-5) in mg/cm<sup>2</sup>, spatially-constant value when

VARIA0N = "NEGLECT"

RESEXP = exponent n in Eq. (5-5), spatially-constant value when VARIA0N =

"NEGLECT"

EXPM = exponent m in Eq. (5-5)

VARIAON = "INCLUDE" - spatially-variable values of a<sub>0</sub> and n in Eq. (5-5), input

from a0\_init and exp\_init files

"NEGLECT" - spatially-constant values of a<sub>0</sub> and n in Eq. (5-5), input as

A0IN and RESEXP

7. <u>Comment - Cohesive Sediment Bed Property Parameters</u>

80 COM 80A1

COM = user specified comment for cohesive sediment bed property parameters

8. <u>Cohesive Sediment Bed Property Parameters</u>

 10
 20
 30
 40
 50
 60

 DENCOH
 VARIBULK
 P0(1)
 VARIPO
 BFCOH
 Z0COH

F10.0, 3X,A7, F10.0,3X,A7,2F10.0

DENCOH = bulk density of cohesive sediment bed in g/cm<sup>3</sup>

VARIBULK = "INCLUDE" - spatially-variable sediment bed bulk density (g/cm<sup>3</sup>), input



from bed bulkden file

"NEGLECT" - spatially-constant bulk density, input as DENCOH

(cohesive bed) and DENNON (non-cohesive bed)

NOTE: If SEDTYPE = "BOTH", then VARIBULK must have same values in both

co\_sed.inp and non coh\_sed.inp.

P0(1) = initial, spatially-constant fraction of fine class sediment in bed

VARIPO = "INCLUDE" - initial, spatially-variable fraction of fine class sediment in

bed, input from p0\_init file

"NEGLECT" - initial, spatially-constant fraction of fine class sediment in

bed, input as P0(1)

BFCOH = bottom friction coefficient for cohesive sediments (non-dimensional)

Z0COH = bottom roughness coefficient for cohesive sediments, in meters

# 9. Comment - Cohesive Bed Consolidation Parameters

80 COM 80A1

COM = user specified comment for cohesive bed consolidation parameters

#### 10. <u>Cohesive Bed Consolidation Parameters</u>

10	20	30	40	50	60	70
FTIME(1)	FTIME(2)	FTIME(3)	FTIME(4)	FTIME(5)	FTIME(6)	FTIME(7)
8F10.0						

FTIME(1) = time after deposition of sediment layer 1, in days time after deposition of sediment layer 2, in days FTIME(2) = FTIME(3) =time after deposition of sediment layer 3, in days time after deposition of sediment layer 4, in days FTIME(4) = FTIME(5) = time after deposition of sediment layer 5, in days FTIME(6) = time after deposition of sediment layer 6, in days FTIME(7) time after deposition of sediment layer 7, in days

# 11. <u>Comment - Initial Cohesive Bed Thickness</u>

\_\_\_\_\_\_80 COM

80A1

COM = user specified comment for cohesive bed thickness



#### 12. <u>Initial Cohesive Bed Thickness</u>

TSED0(1) TSED0(2) TSED0(3) TSED0(4) TSED0(5) TSED0(6) TSED0(7)	10	20	30	40	50	60	70
	TSED0(1)	TSED0(2)	TSED0(3)	TSED0(4)	TSED0(5)	TSED0(6)	TSED0(7)

8F10.0

TSED0(1) = initial thickness of sediment layer 1, in cm
TSED0(2) = initial thickness of sediment layer 2, in cm
TSED0(3) = initial thickness of sediment layer 3, in cm
TSED0(4) = initial thickness of sediment layer 4, in cm
TSED0(5) = initial thickness of sediment layer 5, in cm
TSED0(6) = initial thickness of sediment layer 6, in cm
TSED0(7) = initial thickness of sediment layer 7, in cm

# 13. <u>Comment - Cohesive Bed Critical Shear Stress</u>

COM = user specified comment for critical shear stress

# 14. <u>Cohesive Bed Critical Shear Stress</u>

10	20	30	40	50	60	70
TAUCR(1)	TAUCR(2)	TAUCR(3)	TAUCR(4)	TAUCR(5)	TAUCR(6)	TAUCR(7)
1710011(1)	1710011(2)	1710011(0)	1710011(1)	1710011(0)	1710011(0)	171001

8F10.0

TAUCR(1)	=	critical shear stress of sediment layer 1, in dynes/cm <sup>2</sup>
TAUCR(2)	=	critical shear stress of sediment layer 2, in dynes/cm <sup>2</sup>
TAUCR(3)	=	critical shear stress of sediment layer 3, in dynes/cm <sup>2</sup>
TAUCR(4)	=	critical shear stress of sediment layer 4, in dynes/cm <sup>2</sup>
TAUCR(5)	=	critical shear stress of sediment layer 5, in dynes/cm <sup>2</sup>
TAUCR(6)	=	critical shear stress of sediment layer 6, in dynes/cm <sup>2</sup>
TAUCR(7)	=	critical shear stress of sediment layer 7, in dynes/cm <sup>2</sup>

# 15. <u>Comment - Initial Suspended Sediment Concentration</u>

COM = user specified comment for initial suspended sediment concentration



16. <u>Initial Suspended Sediment Concentration</u>

10 CSI F10.0

CSI = initial, spatially-constant cohesive sediment concentration, in mg/l

17. Comment - Cohesive Sediment Concentrations at Open Boundaries

10 COM 80A1

COM = user specified comment for cohesive sediment concentrations at open boundaries

18. Number of Grid Elements

NUMEBSCE 15

NUMEBCSE = total number of open boundary elements at which cohesive sediment concentrations will be specified

19. <u>Time of Observation</u>

10 TIME F10.1

TIME = time in hours = 0.0 for initial time

20. <u>Location of Grid Elements and Cohesive Sediment Data</u>

 5
 10
 15
 20
 25

 ISEED
 JSEED
 ISEEC
 JSEEC
 CBDRYSL(1)
 ... CBDRYSL(IKSL)

4I5,100F5.0

ISEED = i number of grid element where cohesive sediment is specified



JSEED = j number of grid element where cohesive sediment is specified

ISEEC = i number of connecting grid element (nearest interior non-boundary grid

element)

JSEEC = j number of connecting grid element (nearest interior non-boundary grid

element)

CBDRYSL = cohesive sediment concentration in mg/l at "TIME" for each standard

level (not sigma level)

NOTE:

- 1. Sequence (ISEED/JSEED/ISEEC/JSEEC/ CBDRYSL) is repeated for each location. Total number = NUMEBCSE (total number of boundary grid elements). The sequence (TIME/CBDRYSL) is repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs. "TIME" for cohesive sediment observations need not be the same as for elevation observations in run\_data.
- 2. If HYDTYPE = 'INTERNAL', then NUMEBCSE = NUMEBC (as specified in Data Group F, Table 8-3B: Open Boundary Condition Information in run\_data).
- 3. If HYDTYPE = 'EXTERNAL', then cohesive sediment concentrations **must** be specified at all open boundaries in the domain.

#### 21. Comment - Cohesive Sediment Concentrations at River Discharges

COM = user specified comment for cohesive sediment concentrations at river discharges

#### 22. Number of Grid Elements

NUMQBCSE = total number of river discharges at which cohesive sediment concentrations will be specified

# 23. <u>Location of Grid Elements</u>

	5	10	15	20
	ISEQD	JSEQD	ISEQC	JSEQC
415				



ISEQD = i number of grid element discharge enters JSEQD = j number of grid element discharge enters

ISEQC = i number of connecting exterior boundary grid element JSEQC = j number of connecting exterior boundary grid element

NOTE: Sequence ISEQD/JSEQD/ISEQC/JSEQC is repeated for each discharge

location.

# 24. <u>Time of Observation</u>

\_\_\_\_\_10

F10.1

TIME = time in hours

= 0.0 for initial time

# 25. Cohesive Sediment Data

	10	20	30	80_
C	DIS(1)	CDIS(2)	CDIS(3)	CDIS(NUMQBCSE)

8F10.1

CDIS = cohesive sediment concentration of river discharge in mg/l

NOTE:

- 1. The sequence (TIME/CDIS) is repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs. Discharges leaving the mode domain (shore-based intakes) do not require associated CDIS values. However, a value of zero should be input for CDIS of these discharges.
- 2. If HYDTYPE = 'INTERNAL', then NUMQBCSE = NUMQBC (as specified in Data Group G, Table 8-3B: Discharge Information in run\_data).
- 3. If HYDTYPE = 'EXTERNAL', then cohesive sediment concentrations **must** be specified at all river discharges in the domain.

NOTE:

"TIME" for all the above boundary conditions is absolute time measured from beginning of COLD START run and incremented with each subsequent HOT START run.



26. Comment - Cohesive Sediment Loading in Diffuser Discharges

80 COM 80A1

COM = user specified comment for cohesive sediment loading in diffuser discharges

27. Number of Grid Elements

NUMDBCSE = total number of diffusers at which cohesive sediment loading will be specified. If NUMDBCSE = 0, then terminate input.

28. <u>Location of Grid Elements/Vertical Distribution of Diffuser Loadings</u>

5	10	15	20	110
IDDSE(NUMDBCSE)	JDDSE(NUMDBCSE)	VDDISTSE(1)	VDDISTSE(2)	VDDISTSE(KBM1)

2I5,20F5.0

IDDSE = i number of grid element diffuser enters/leaves JDDSE = j number of grid element diffuser enters/leaves

VDDISTSE = percentage (not fraction) of total diffuser loading CDIFF apportioned in

each model layer from surface to bottom at location (IDDSE, JDDSE)

KBM1 = KB-1

NOTE: 1. Sequence (IDDSE/JDDSE/VDDISTSE) is repeated for each diffuser

2. More than one diffuser can be specified at the same location (IDDSE,

JDDSE)

29. <u>Time of Observation</u>

10 TIME F10.5



# 10.0 Model Input Data Structure

TIME = time in hours

= 0.0 for initial time

NOTE: TIME is absolute time measured from beginning of COLD START run and

incremented with each subsequent HOT START run.

# 30. <u>Diffuser Loading Data</u>

10	20	 80
CDIFF(1)	CDIFF(2)	 CDIFF(NUMDBCSE)
8F10.5		

CDIFF = diffuser loading in kg/day.

NOTE: Sequence (TIME/CDIFF) repeated for each observation. Final "TIME" must

be greater than (NSTEPS\*DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPSxDTI)/3600 for HOT

 $START \ runs.$ 



## Table 10-9. noncoh\_sed.inp INPUT FILE

NOTE: This file must be included for non-cohesive sediment transport simulations. (SEDTRAN = "INCLUDE" and SEDTYPE = "BOTH" or "SAND")

1. <u>Comment - Sediment Transport Control Parameters</u>

COM = user specified comment for sediment transport control parameters

2. <u>Sediment Transport Control Parameters</u>

NSEDBEG = time step at which to start sediment transport calculation

NSBED = frequency, in time steps, at which to calculate deposition/ resuspension

fluxes

NOTE: If SEDTYPE = "BOTH", then NSEDBEG and NSBED must have the same

values in both coh\_sed.inp and noncoh\_sed.inp.

3. Comment - Non-Cohesive Sediment Transport Parameters

COM = user specified comment for non-cohesive sediment transport parameters

4. Non-Cohesive Sediment Transport Parameters

10	20	30	40	50
WS2	DENNON	VARIBULK	SUSARM	BEDTHI

2F10.0,3X,A7,2F10.0

WS2 = settling speed of non-cohesive sediment, in  $\mu$ m/s DENNON = bulk density of non-cohesive sediment bed, in g/cm<sup>3</sup>

VARIBULK = "INCLUDE" - spatially-variable sediment bed bulk density (g/cm<sup>3</sup>), input

from bed\_bulkden file



"NEGLECT" - spatially-constant bulk density, input as DENCOH

(cohesive bed) and DENNON (non-cohesive bed)

SUSARM = non-cohesive bed armoring constant (0 - 1.0 range)

NOTE: If SEDTYPE = "BOTH", then VARIBULK must have same values for both

coh\_sed.inp and noncoh\_sed.inp

BEDTHI = initial thickness of non-cohesive bed, in cm

5. <u>Comment - Initial Suspended Sediment Concentration</u>

COM = user specified comment for initial suspended sediment concentration

6. <u>Initial Suspended Sediment Concentration</u>

CSI = initial, spatially-constant non-cohesive sediment concentration, in mg/l

7. Comment - Non-Cohesive Sediment Concentrations at Open Boundaries

COM = user specified comment for non-cohesive sediment concentrations at open boundaries

8. Number of Grid Elements

NUMEBCSE = total number of open boundary elements at which non-cohesive sediment concentrations will be specified

#### 9. Time of Observation

10 TIME F10.1

TIME = time in hours

= 0.0 for initial time

#### 10. Location of Grid Elements and Non-Cohesive Sediment Data

5	10	15	20	25	
ISEED	JSEED	ISEEC	JSEEC	CBDRYSL(1)	CBDRYSL(IKSL)
4I5 100F5 0					

415,100F5.C

**ISEED** = i number of grid element where non-cohesive sediment is specified

**JSEED** = j number of grid element where non-cohesive sediment is specified **ISEEC** 

= i number of connecting grid element (nearest interior non-boundary grid

**JSEEC** = i number of connecting grid element (nearest interior non-boundary grid

element)

**CBDRYSL** = non-cohesive sediment concentration in mg/l at "TIME" for each standard

level (not sigma level)

NOTE:

- 1. Sequence (ISEED/JSEED/ISEEC/JSEEC/ CBDRYSL) is repeated for each location. Total number = NUMEBCSE (total number of boundary grid elements). The sequence (TIME/CBDRYSL) is repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs. "TIME" for noncohesive sediment observations need not be the same as for elevation observations in run data.
- 2. If HYDTYPE = 'INTERNAL', then NUMEBCSE = NUMEBC (as specified in Data Group F, Table 8-3B: Open Boundary Condition Information in run\_data).
- 3. If HYDTYPE = 'EXTERNAL', then non-cohesive sediment concentrations must be specified at all open boundaries in the domain.

#### 11. Comment - Non-Cohesive Sediment Concentrations at River Discharges

10 COM 80A1



COM = user specified comment for non-cohesive sediment concentrations at river discharges

# 12. <u>Number of Grid Elements</u>

NUMQBCSE = total number of river discharges at which non-cohesive sediment concentrations will be specified

# 13. <u>Location of Grid Elements</u>

	5	10	15	20	
	ISEQD	JSEQD	ISEQC	JSEQC	
4	·15				

ISEQD = i number of grid element discharge enters JSEQD = j number of grid element discharge enters

ISEQC = i number of connecting exterior boundary grid element JSEQC = j number of connecting exterior boundary grid element

NOTE: Sequence ISEQD/JSEQD/ISEQC/JSEQC is repeated for each discharge location.

# 14. Time of Observation

TIME = time in hours = 0.0 for initial time

# 15. <u>Non-cohesive Sediment Data</u>

10	20	30	80
CDIS(1)	CDIS(2)	CDIS(3)	CDIS(NUMQBCSE)
8F10 1			

CDIS = non-cohesive sediment concentration of river discharge in mg/l

NOTE: 1. The sequence (TIME/CDIS) is repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the



run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs. Discharges leaving the mode domain (shore-based intakes) do not require associated CDIS values. However, a value of zero should be input for CDIS of these discharges.

- 2. If HYDTYPE = 'INTERNAL', then NUMQBCSE = NUMQBC (as specified in Data Group G, Table 8-3B: Discharge Information in run\_data).
- 3. If HYDTYPE = 'EXTERNAL', then non-cohesive sediment concentrations **must** be specified at all river discharges in the domain.

NOTE: "TIME" for all the above boundary conditions is absolute time measured from beginning of COLD START run and incremented with each subsequent HOT START run.

# 16. Comment - Non-cohesive Sediment Loading in Diffuser Discharges

COM = user specified comment for non-cohesive sediment loading in diffuser discharges

#### 17. Number of Grid Elements

NUMDBCSE = total number of diffusers at which non-cohesive sediment loading will be specified. If NUMDBCSE = 0, then terminate input.

# 18. <u>Location of Grid Element/Vertical Distribution of Diffuser Loadings</u>

5	10	15	20	 110
IDDSE(NUMDBCSE)	JDDSE(NUMDBCSE)	VDDISTSE(1)	VDDISTSE(2)	VDDISTSE(KBM1)
2l5,20F5.0				

IDDSE = i number of grid element diffuser enters/leaves

JDDSE = j number of grid element diffuser enters/leaves

VDDISTSE = percentage (not fraction) of total diffuser loading CDIFF apportioned in

each model layer from surface to bottom at location (IDDSE, JDDSE)

KBM1 = KB-1



NOTE:

- 1. Sequence (IDDSE/JDDSE/VDDISTSE) is repeated for each diffuser
- 2. More than one diffuser can be specified at the same location (IDDSE, JDDSE)

# 19. <u>Time of Observation</u>

TIME = time in hours

= 0.0 for initial time

NOTE: TIME is absolute time measured from beginning of COLD START run and

incremented with each subsequent HOT START run.

# 20. <u>Diffuser Loading Data</u>

10	20	 80
CDIFF(1)	CDIFF(2)	 CDIFF(NUMDBCSE)
8F10.5		

CDIFF = diffuser loading in kg/day.

NOTE: Sequence (TIME/CDIFF) repeated for each observation. Final "TIME" must

be greater than (NSTEPS\*DTI)/3600 (the duration of the run), for COLD START runs, and greater than 1END + (NSTEPSxDTI)/3600 for HOT

START runs.



# Table 10-10. coh\_trace.inp INPUT FILE

NOTE: This file must be included for cohesive sediment-bound transport simulations.

(CHEMTRAN = "INCLUDE", SEDTRAN = "INCLUDE" and SEDTYPE

= "BOTH" or "MUD ")

1. <u>Comment - Sediment-Bound Transport Control Parameters</u>

COM = user specified comment for sediment-bound transport control parameters

2. Sediment-Bound Transport Control Parameters

10	20	30	40	50
CHEMI(1)	NCHEMLAY	CHEMTHIK	CHEMACT	CHEMDRAT

F10.0, I10, 4F10.0

CHEMI(1) = initial, spatially-constant, cohesive sediment-bound concentration (water

column), in  $\mu$ g/l

NCHEMLAY = number of layers in sediment-bound tracer bed model

CHEMTHIK = thickness of layers in sediment-bound tracer bed model, in cm CHEMACT = active layer thickness, in cm (CHEMACT ≥ CHEMTHIK) CHEMDRAT = sediment-bound tracer decay rate (first-order decay), in day<sup>-1</sup>

NOTE: NCHEMLAY, CHEMTHIK and CHEMACT must have the same values in

both coh\_trace.inp and noncoh\_trace.inp

3. <u>Comment - Cohesive Sediment-Bound Tracer Concentrations at Open Boundaries</u>

10 COM 80A1

COM = user specified comment for cohesive sediment-bound tracer

concentrations at open boundaries



# 4. <u>Number of Grid Elements</u>

NUMEBCCH

NUMEBCCH = total number of open boundary elements at which cohesive sediment-bound tracer concentrations will be specified

# 5. <u>Time of Observation</u>

10 COM 80A1

TIME = time in hours = 0.0 for initial time

### 6. <u>Location of Grid Elements and Cohesive Sediment-Bound Tracer Data</u>

5 15 20 25 **ICHED JCHED ICHEC JCHEC** CBDRYSL(1) ... CBDRYSL(IKSL) 4I5,100F5.0 **ICHED** i number of grid element where cohesive sediment is specified j number of grid element where cohesive sediment is specified **ICHED ICHEC** i number of connecting grid element (nearest interior non-boundary grid element) **JCHEC** i number of connecting grid element (nearest interior non-boundary grid element) = **CBDRYSL** cohesive sediment-bound tracer concentration in  $\mu$ g/l at "TIME" for each standard level (not sigma level) NOTE: Sequence (ICHED/JCHED/ICHEC/JCHEC/ CBDRYSL) is repeated 1. for each location. Total number = NUMEBCCH (total number of boundary grid elements). The sequence (TIME/CBDRYSL) is repeated for each observation. Final "TIME" must be greater than (NSTEPS x

elevation observations in run data.

DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs. "TIME" for cohesive tracer observations need not be the same as for



- 2. If HYDTYPE = 'INTERNAL', then NUMEBCCH = NUMEBC (as specified in Data Group F, Table 8-3B: Open Boundary Condition Information in run\_data).
- 3. If HYDTYPE = 'EXTERNAL', then cohesive sediment-bound tracer concentrations **must** be specified at all open boundaries in the domain.
- 7. Comment Cohesive Sediment-Bound Tracer Concentrations at River Discharges

COM = user specified comment for cohesive sediment-bound tracer concentrations at river discharges

8. Number of Grid Elements

NUMQBCCH = total number of river discharges at which cohesive sediment-bound tracer concentrations will be specified

9. <u>Location of Grid Elements</u>

	5		10	15	20
	ICHQD	JC	CHQD	ICHQC	JCHQC
415					

ICHQD = i number of grid element discharge enters

JCHQD = j number of grid element discharge enters

ICHQC = i number of connecting exterior boundary grid element

JCHQC = j number of connecting exterior boundary grid element

NOTE: Sequence ICHQD/JCHQD/ICHQC/JCHQC is repeated for each discharge location.

10. <u>Time of Observation</u>



TIME = time in hours = 0.0 for initial time

#### 11. Cohesive Sediment-Bound Tracer Data

10	20	30	80
CDIS(1)	CDIS(2)	CDIS(3)	CDIS(NUMQBCCH)
8F10.1			

**3.** ..

CDIS = cohesive sediment-bound tracer concentration of river discharge in  $\mu g/l$ 

NOTE:

- 1. The sequence (TIME/CDIS) is repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs. Discharges leaving the mode domain (shore-based intakes) do not require associated CDIS values. However, a value of zero should be input for CDIS of these discharges.
- 2. If HYDTYPE = 'INTERNAL', then NUMQBCCH = NUMQBC (as specified in Data Group G, Table 8-3B: Discharge Information in run\_data).
- 3. If HYDTYPE = 'EXTERNAL', then cohesive sediment-bound tracer concentrations **must** be specified at all river discharges in the domain.

NOTE:

"TIME" for all the above boundary conditions is absolute time measured from beginning of COLD START run and incremented with each subsequent HOT START run.

#### 12. Comment - Cohesive Sediment-Bound Tracer Loading in Diffuser Discharges

80 COM 80A1

COM = user specified comment for cohesive sediment-bound tracer loading in diffuser discharges

#### 13. Number of Grid Elements

NUMDBCCH



NUMDBCCH = total number of diffusers at which cohesive sediment-bound tracer loading will be specified. If NUMDBCCH = 0, then terminate input.

### 14. <u>Location of Grid Elements/Vertical Distribution of Diffuser Loadings</u>

2I5,20F5.0

IDDCH = i number of grid element diffuser enters/leaves JDDCH = j number of grid element diffuser enters/leaves

VDDISTCH = percentage (not fraction) of total diffuser loading CDIFF apportioned

in each model layer from surface to bottom at location (IDDCH,

JDDCH)

KBM1 = KB-1

NOTE: 1. Sequence (IDDCH/JDDCH/VDDISTCH) is repeated for each diffuser.

2. More than one diffuser can be specified at the same location (IDDCH, JDDCH).

### 15. <u>Time of Observation</u>

TIME = time in hours

= 0.0 for initial time

NOTE: TIME is absolute time measured from beginning of COLD START run and

incremented with each subsequent HOT START run.

### 16. <u>Diffuser Loading Data</u>

10	20	 80
CDIFF(1)	CDIFF(2)	 CDIFF(NUMDBCCH)
8F10.5		



CDIFF = diffuser loading in kg/day

NOTE: Sequence (TIME/CDIFF) repeated for each observation. Final "TIME" must

be greater than (NSTEPS \* DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT

START runs.



#### Table 10-11. noncoh\_trace.inp INPUT FILE

NOTE:

This file must be included for non-cohesive sediment-bound transport simulations. (CHEMTRAN = "INCLUDE", SEDTRAN = "INCLUDE" and SEDTYPE = "BOTH" or "SAND")

1. <u>Comment - Sediment-Bound Transport Control Parameters</u>



COM = user specified comment for sediment-bound transport control parameters

2. <u>Sediment-Bound Transport Control Parameters</u>

10	20	30	40	50
CHEMINIT	NCHEMLAY	CHEMTHIK	CHEMACT	CHEMDRAT

F10.0, I10, 4F10.0

CHEMINIT = initial, spatially-constant, non-cohesive sediment-bound concentration

(water column), in  $\mu$ g/l

NCHEMLAY = number of layers in sediment-bound tracer bed model

CHEMTHIK = thickness of layers in sediment-bound tracer bed model, in cm CHEMACT = active layer thickness, in cm (CHEMACT ≥ CHEMTHICK)

CHEMDRAT = non-cohesive sediment-bound tracer decay rate (first-order decay), in

dav-1

NOTE: NCHEMLAY, CHEMTHIK and CHEMACT must have the same values in

both coh\_trace.inp and noncoh\_trace.inp

3. <u>Comment - Non-Cohesive Sediment-Bound Tracer Concentrations at Open Boundaries</u>

COM

= user specified comment for non-cohesive sediment-bound tracer concentrations at open boundaries



# 4. <u>Number of Grid Elements</u>

NUMEBCCH = total number of open boundary elements at which non-cohesive sediment-bound tracer concentrations will be specified

# 5. Time of Observation

TIME = time in hours = 0.0 for initial time

# 6. <u>Location of Grid Elements and Non-Cohesive Sediment-Bound Tracer Data</u>

5	10	15	20	25	
ICHED	JCHED	ICHEC	JCHEC	CBDRYSL(1)	CBDRYSL(IKSL)
4I5,100F5.0					

ICHED	=	i number of grid element where non-cohesive tracer is specified
JCHED	=	j number of grid element where non-cohesive tracer is specified
ICHEC	=	u number of connecting grid element (nearest interior non-boundary grid
		element)
JCHEC	=	j number of connecting grid element (nearest interior non-boundary grid
		element)
CBDRYSL	=	non-cohesive sediment-bound tracer concentration in $\mu$ g/l at "TIME"
		for each standard level (not sigma level)

NOTE:

- 1. Sequence (ICHED/JCHED/ICHEC/JCHEC/ CBDRYSL) is repeated for each location. Total number = NUMEBCCH (total number of boundary grid elements). The sequence (TIME/CBDRYSL) is repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs. "TIME" for non-cohesive tracer observations need not be the same as for elevation observations in run data.
- 2. If HYDTYPE = 'INTERNAL', then NUMEBCCH = NUMEBC (as specified in Data Group F, Table 8-3B: Open Boundary Condition Information in run\_data).
- 3. If HYDTYPE = 'EXTERNAL', then non-cohesive sediment-bound tracer concentrations **must** be specified at all open boundaries in the domain.
- 7. <u>Comment Non-Cohesive Sediment-Bound Tracer Concentrations at River Discharges</u>

COM

= user specified comment for non-cohesive sediment-bound tracer concentrations at river discharges

#### 8. Number of Grid Elements

NUMQBCCH = total number of river discharges at which non-cohesive sediment-bound tracer concentrations will be specified

#### 9. Location of Grid Elements

5	10	15	20
ICHQD	JCHQD	ICHQC	JCHQC
415			

ICHQD = i number of grid element discharge enters JCHQD = j number of grid element discharge enters

ICHQC = i number of connecting exterior boundary grid element



JCHQC = j number of connecting exterior boundary grid element

<u>NOTE</u>: Sequence ICHQD/JCHQD/ICHQC/JCHQC is repeated for each discharge

location.

#### 10. Time of Observation

TIME = time in hours = 0.0 for initial time

#### 11. Non-Cohesive Sediment-Bound Tracer Data

	10	20	30	
_	CDIS(1)	CDIS(2)	CDIS(3)	CDIS(NUMQBCCH)

8F10.1

**CDIS** 

= non-cohesive sediment-bound tracer concentration of river discharge in  $\mu$ g/l

NOTE:

- 1. The sequence (TIME/CDIS) is repeated for each observation. Final "TIME" must be greater than (NSTEPS x DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT START runs. Discharges leaving the mode domain (shore-based intakes) do not require associated CDIS values. However, a value of zero should be input for CDIS of these discharges.
- 2. If HYDTYPE = 'INTERNAL', then NUMQBCCH = NUMQBC (as specified in Data Group G, Table 8-3B: Discharge Information in run\_data).
- 3. If HYDTYPE = 'EXTERNAL', then non-cohesive sediment-bound tracer concentrations **must** be specified at all river discharges in the domain.

NOTE:

"TIME" for all the above boundary conditions is absolute time measured from beginning of COLD START run and incremented with each subsequent HOT START run.



12. Comment - Non-Cohesive Sediment-bound Tracer Loading in Diffuser Discharges

COM = user specified comment for non-cohesive sediment-bound tracer loading in diffuser discharges

13. Number of Grid Elements

NUMDBCCH = total number of diffusers at which non-cohesive sediment-bound tracer loading will be specified. If NUMDBCCH = 0, then terminate input.

14. Location of Grid Elements/Vertical Distribution of Diffuser Loadings

5	10	15
IDDCH(NUMDBCH)	JDDCH(NUMDBCCH)	VDDISTCH(1)

215,20F5.0

IDDCH = i number of grid element diffuser enters/leaves JDDCH = j number of grid element diffuser enters/leaves

VDDISTCH = percentage (not fraction) of total diffuser loading CDIFF apportioned in

each model layer from surface to bottom at location (IDDCH, JDDCH)

KBM1 = KB-1

NOTE: 1. Sequence (IDDCH/JDDCH/VDDISTCH) is repeated for each diffuser.

2. More than one diffuser can be specified at the same location (IDDCH, JDDCH).

15. Time of Observation

\_\_\_\_\_\_10 \_\_\_\_\_TIME F10.5



### 10.0 Model Input Data Structure

TIME = time in hours

= 0.0 for initial time

NOTE: TIME is absolute time measured from beginning of COLD START run and

incremented with each subsequent HOT START run.

# 16. <u>Diffuser Loading Data</u>

10	20	 80
CDIFF(1)	CDIFF(2)	 CDIFF(NUMDBCCH)
8F10.5		

CDIFF =  $\frac{\text{diffuser loading in kg/day.}}{\text{diffuser loading in kg/day.}}$ 

NOTE: Sequence (TIME/CDIFF) repeated for each observation. Final "TIME" must

be greater than (NSTEPS \* DTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEPS x DTI)/3600 for HOT

 $START\ runs.$ 



# Table 10-12. partrack.inp INPUT FILE

<u>NOTE</u>: This file must be included for particle tracking simulations. (PARTICLE = "INCLUDE")

# 1. <u>Comment - Particle Tracking Input Parameters</u>

10 COM 80A1

COM = user specified comment for particle tracking input parameters

### 2. Particle Tracking Input Parameters

8	16	24	32	40
NFREQ	NPART	IRELST	IRELEND	NSOURCE

618

NFREQ = number of time steps between each particle release

NPART = number of particles per release IRELST = time step of first particle release IRELEND = time step of last particle release NSOURCE = number of particle sources

#### 3. <u>Particle Source Locations</u>

 8
 16
 24

 ISOURCE(M)
 JSOURCE(M)
 KSOURCE(M)

318

ISOURCE(M) = i number of grid element for particle source M JSOURCE(M) = j number of grid element for particle source M KSOURCE(M) = k number of grid element for particle source M



NOTE:

- 1. There must be M = 1, ..., NSOURCE lines specified after line 2 for the particle source locations.
- 2. The corner\_loc file is needed for particle tracking.



# Table 10-13. bed\_mask INPUT FILE

NOTE: This file must be included for all sediment transport simulations.(SEDTRAN = "INCLUDE")

Input sediment bed map for the model grid as follows:

DO 10 I = 1, IM READ (5,20) (IBMSK(I,J), J= 1, JM)

CONTINUE 10 20

FORMAT (40I3)

**IBMSK** = 0, cohesive sediment element

1, non-cohesive sediment element with suspended transport

-1, hard bottom (no suspended transport)



# Table 10-14. p0\_init INPUT FILE

 $\underline{NOTE}$ : Include this file only if SEDTRAN = "INCLUDE", SEDTYPE = "BOTH" or "MUD", and VARIP0 = 'INCLUDE'

Input spatially-variable, sediment bed bulk density for the model grid as follows:

DO 10 I = 1, IM READ (5,20) (PINIT(I,J), J= 1, JM)

- 10 CONTINUE
- 20 FORMAT (20F6.2)

PINIT = fraction of sediment bed initially composed of cohesive sediment

NOTE: only specify PINIT for cohesive elements, IBMSK = 0



# Table 10-15. a0\_init INPUT FILE

Include this file only if SEDTRAN = "INCLUDE", SEDTYPE = "BOTH" or "MUD" and NOTE: VARIAON = 'INCLUDE'

Input spatially-variable a<sub>o</sub> values for the model grid as follows:

- 10
- 20 FORMAT (8E10.3)

Α0 a<sub>0</sub> value, for erosion potential in mg/cm<sup>2</sup>

NOTE: only specify A0 for cohesive elements, IBMSK = 0



# Table 10-16. exp\_init INPUT FILE

NOTE: Include this file only if SEDTRAN = "INCLUDE", SEDTYPE = "BOTH" or "MUD", and VARIA0N = 'INCLUDE'

Input spatially-variable exponent n values for the model grid as follows:

DO 10 I = 1, IM READ (5,20) (REXP(I,J), J= 1, JM) CONTINUE

10 CONTINUE 20 FORMAT (8E10.3)

REXP = exponent n, for erosion potential in mg/cm<sup>2</sup>

NOTE: only specify REXP for cohesive elements, IBMSK = 0



# Table 10-17. bed\_d50 INPUT FILE

<u>NOTE</u>: Include this file only if non-cohesive suspended transport is simulated (SEDTRAN =

"INCLUDE", SEDTYPE = "BOTH" or "SAND" and IBMSK = 1 for some elements in

bed\_mask)

Input spatially-variable D<sub>50</sub> values for the model grid as follows:

DO 10 I = 1, IM

READ (5,20) (D50VAR(I,J), J= 1, JM)

10 CONTINUE

20 FORMAT (20F6.0)

D50VAR = median grain size of non-cohesive sediment ( $D_{50}$ ), in microns

NOTE: only specify  $D_{50}$  for non-cohesive elements, IBMSK = 1



### Table 10-18. bed\_frac.mud INPUT FILE

<u>NOTE</u>: Include this file only if non-cohesive suspended transport is simulated (SEDTRAN =

"INCLUDE", SEDTYPE = "BOTH" or "SAND" and IBMSK = 1 for some elements in

bed\_mask)

Input spatially-variable, initial non-cohesive bed fractions for the model grid as follows:

DO 10 I = 1, IM READ (5,20) (FPBED(I,J), J= 1, JM)

10 CONTINUE

20 FORMAT (20F6.3)

FPBED = fraction of sediment bed initially composed of suspended non-cohesive

sediment, this is the clay/silt fraction in the bed.

 $\underline{NOTE}$ : only specify FPBED for non-cohesive elements, IBMSK = 1



### Table 10-19. bed\_frac.sand INPUT FILE

<u>NOTE</u>: Include this file only if non-cohesive suspended transport is simulated (SEDTRAN =

"INCLUDE", SEDTYPE = "BOTH" or "SAND" and IBMSK = 1 for some elements in

bed\_mask)

Input spatially-variable, initial non-cohesive bed fractions for the model grid as follows:

DO 10 I = 1, IM READ (5,20) (FPBED(I,J), J= 1, JM)

10 CONTINUE

20 FORMAT (20F6.3)

FPBED = fraction of sediment bed initially composed of suspended non-cohesive

sediment, this is the fine sand fraction in the bed.

 $\underline{NOTE}$ : only specify FPBED for non-cohesive elements, IBMSK = 1



# Table 10-20. bed\_bulkden INPUT FILE

NOTE: Include this file only if SEDTRAN = "INCLUDE", SEDTYPE = "BOTH" or "MUD", and VARIBULK = 'INCLUDE'

Input spatially-variable, sediment bed bulk density for the model grid as follows:

DO 10 I = 1, IM READ (5,20) (CBED(I,J), J= 1, JM) 10 CONTINUE 20 FORMAT (20F6.2)

CBED = sediment bed bulk density  $(g/cm^3)$ 



# Table 10-21. bed\_chemic INPUT FILE

NOTE: Include this file only if SEDTRAN = "INCLUDE" and CHEMTRAN = 'INCLUDE'

Input spatially-variable, initial bed concentration of sediment-bound tracer for the model grid as follows:

DO 10 N = 1, NCHEMLAY
DO 10 I = 1, IM

READ (5,20) (CBEDCHEM (N,I,J),J=1,JM)
CONTINUE
FORMAT (10F8.0)

CBEDCHEM(N) = initial bed concentration of sediment-bound tracer in layer N ( $\mu$ g tracer/g sediment)



### Table 10-22. hqi\_geom INPUT FILE (UNFORMATTED)

READ(199) Z,ZZ,DZ,DZZ READ(199) H1,H2,H,ANG READ(199) ICNT READ(199) (INDX(I), I = 1,ICNT) READ(199) (JNDX(I), I =1,ICNT)

**Unit 199** "hqi\_geom" Z depth of the interface between sigma levels ZZ0.5 (Z(k) + Z(k+1))DZthickness of the sigma level average depth of the grid element (m) DZZdistance in the  $\xi_1$  direction at the center of the grid (m) H1 distance in the  $\xi_2$  direction at the center of the grid (m) H2 = Н water depth (m) ANG = angle between east and the  $\xi_1$  direction measured in a counter-clockwise direction **ICNT** total number of water elements in horizontal plane == i number of water element I INDX(I) JNDX(I) j number of water element I



#### Table 10-23. hqi\_tran INPUT FILE (UNFORMATTED)

```
READ (IUTRN) TMIDDLE
READ (IUTRN) HPRNU
READ (IUTRN) ((WETGU(I,K),I=1,ICNT), K=1,KBM1)
READ (IUTRN) ((WETGV(I,K),I=1,ICNT), K=1,KBM1)
READ (IUTRN) ((WETGW(I,K),I=1,ICNT), K=1,KBM1)
READ (IUTRN) ((WETGAAM(I,K),I=1,ICNT), K=1,KBM1)
READ (IUTRN) ((WETGKH(I,K),I=1,ICNT), K=1,KBM1)
READ (IUTRN) ((WETGKM(I,K),I=1,ICNT), K=1,KBM1)
READ (IUTRN) ((WETGES(I,K),I=1,ICNT), K=1,KBM1)
READ (IUTRN) ((WETGED(I,K),I=1,ICNT), K=1,KBM1)
```

 $IUTRN = 18 ("hqi_tran")$ 

TMIDDLE = time at the middle of the averaging interval (days)

HPRNU = horizontal Prandtl number (momentum mixing/dispersive mixing)

WETGU = low-pass filtered volume flow rate in  $\xi_1$  direction (m<sup>3</sup>/s) WETGV = low-pass filtered volume flow rate in  $\xi_2$  direction (m<sup>3</sup>/s)

WETGW = low-pass filtered vertical volume flow rate (m³/s)
WETGAAM = low-pass filtered horizontal eddy viscosity (m²/s)
WETGKH = low-pass filtered vertical eddy diffusivity (m²/s)
WETGKM = low-pass filtered vertical eddy viscosity (m²/s)

WETGES = initial surface elevation (m)
WETGED = time rate of change of elevation (m/s)



### Table 10-24. wave\_input INPUT FILE (UNFORMATTED)

READ (110) TIME READ (110) WPERIOD READ (110) WHEIGHT READ (110) WDIR

Unit 110 = "wave\_input"

TIME = time at which wave parameters were output (hours)

WPERIOD = mean wave period (seconds)
WHEIGHT = significant wave height (meters)

WDIR = wave direction, measured clockwise from North (degrees)

NOTE: 1. The wave parameters, usually generated by WAM, must be interpolated from the wave model grid to the ECOMSED model grid before storing in "wave\_input."

2. The dimensions of the WPERIOD, WHEIGHT and WDIR arrays are (IM,JM), which is the same as used in ECOMSED.



### Table 10-25. horcon2d.inp INPUT FILE

NOTE: This file must be included if the user specified HORCON (Data Group B.4) as "VARI" (X,A4).

1. Comment - 2-D HORCON Scale Factors

COM = user specified comment for 2-D HORCON scale factors

2. Number of Grid Cells and Base HORCON Value

NVARHF = number of grid cells to be scaled from the base HORCON value HORCON = base HORCON value

3. <u>Comment - Scaling Factors for HORCON</u>

4. <u>2-D HORCON Scale Factors</u>

NOTE: Line 4 should be repeated by NVARHF



#### Table 10-26. Bfric2d.inp INPUT FILE

NOTE: This file must be included if the user specified BFRIC (Data Group B.2) as "VARI".

1. Comment - 2-D Bottom Friction Scale Factors

COM = user specified comment for 2-D bottom friction scale factors

2. Number of Grid Cells and Base Bottom Friction Coefficient

NVARBF = number of grid cells to be scaled from the base bottom friction

coefficient BFRIC

BFRIC = minimum bottom friction coefficient (non-dimensional)

<u>NOTE</u>: ECOMSED will compute its base bottom drag coefficient based on equation (3-

23a) and BFRIC. Then the scaling factors will be applied to the base drag

coefficient.

3. <u>Comment - Scaling Factors for bottom Drag Coefficients</u>

80 COM 80A1



4. <u>2-D Bottom Drag Coefficient Scaling Factors</u>

I, J = grid index

VARBF = bottom drag coefficient scaling factor

NOTE: Line 4 should be repeated by NVARBF



# Table 10-27. umol2d.inp INPUT FILE

NOTE: This file must be included if the user specified UMOL (Data Group B.6) as "VARI" (6X,A4).

1. Comment - 2-D UMOL Scale Factors

COM = user specified comment for 2-D UMOL scale factors

2. Number of Grid Cells and Base UMOL Value

NVARUF = number of grid cells to be scaled from the base UMOL value UMOL = base UMOL value

3. <u>Comment - Scaling Factors for UMOL</u>

4. 2-D UMOL Scale Factors

NOTE: Line 4 should be repeated by NVARUF



# Table 10-28. Z0b2d.inp INPUT FILE

NOTE: This file must be included if the user specified Z0B (Data Group B.1) as "VARI" (6X,A4).

1. <u>Comment - 2-D Z0B Scale Factors</u>

COM = user specified comment for 2-D Z0B scale factors

2. Number of Grid Cells and Base Z0B Value

NVARZ0B = number of grid cells to be scaled from the base Z0B value

Z0B = base Z0B value

3. Comment - Scaling Factors for Z0B

4. 2-D Z0B Scale Factors

NOTE: Line 4 should be repeated by NVARZ0B



### Table 10-29. init\_tracer INPUT FILE

NOTE: This file must be included if the user specified TRICOPT (Table 10-7) as "DATA".

 5	10	15	20	
1	J	CONC1(I,J,1)	CONC1(I,J,2)	 CONC1(I,J,KSL)
		•		<u> </u>

2I5,100F5.0

 $\begin{array}{rcl} I & = & \text{i number of grid element in the } \xi_1 \text{ direction} \\ J & = & \text{j number of grid element in the } \xi_2 \text{ direction} \\ CONC1 & = & \text{dissolved tracer concentration at standard levels} \end{array}$ 

NOTE: KSL = number of standard levels



#### Table 10-30. bed.sdf INPUT FILE

NOTE: This file must be included for sediment transport simulations (if SEDTRAN="INCLUDE" and SEDTYPE="SEDZL]")

1. Comment - Sediment Transport Control Parameters

80 COM 80A1

COM = user specified comments for sediment transport control parameters

2. Sediment Transport Control Parameters

_	10	20	30	40
	NSEDBEG	NSBEDNCHE	Z0BCOH	CFMIN

NSEDBEG = Timestep at which the sediment transport calculations begin.

NSBED = The number of hydrodynamic timesteps between each sediment

transport timestep.

Z0BCOH = The  $Z_0$  of the sediment bed.

CFMIN = The minimum coefficient of friction for the shear stress calculation.

3. Comment - Sediment Bed Control Parameters

80 COM 80A1

COM = user specified comments for sediment bed control parameters

4. Sediment Bed Control Parameters



10	20	30	40
VAR BED	NCALC BL	CONTAU	DEP COEFF

VAR\_BED = Switch for turning on variable sediment bed. If VAR\_BED = 1, then

'core\_field.sdf' is called so that spatial variation in bed properties can

be defined.

NCLAC\_BL = Switch for turning on bedload calculations. If NCLAC\_BL = 1, then bedload transport is calculated, otherwise all material is assumed to transport as suspended load.

CONTAU = If CONTAU is greater than zero, then the number is specified as a

constant shear stress throughout the domain. This is a useful tool for

testing.

DEP COEFF = Fraction of the total sediment mass for a certain size class in a grid box

that can settle in a single time step. Applies to both water-water and

water-sediment settling.

5. Comment - Average Particle Size of Each Size Class

80
СОМ
9011

COM = user specified comments for average particle size of each size class

6. Average Particle Size of Each Size Class

10	20	30	
D50(1)	D50(2)	D50(30	D50(KSED)
8F10.3			

D50 = average particle size,  $D_{50}$ , of each size class ( $\mu$ m) where KSED is the number of size classes.

7. Comment - Critical Shear Stresses for Suspension



80
СОМ
80A1

COM = user specified comments for critical shear stress for suspension

8. Critical Shear Stress for Suspension

10	20	30		
TCRDPS(1)	TCRDPS(2)	TCRDPS(3)	TCRDPS(KSED)	
8F10.3				

TCRCPS = critical shear stress for suspension of each size class in dynes/cm<sup>2</sup>.

9. Comment - Critical Shear Stress for Erosion

10. Critical Shear Stress for Erosion

TAUCRS = critical shear stress for erosion of each size class in dynes/cm<sup>2</sup>.

11. Comment – Average Particle Sizes of the Active Layer



COM = user specified comments for average particle sizes of the active layer

12. Average Particle Sizes of the Active Layer

_	10	20	30	
-	SCLOC(1)	SCLOC(2)	SCLOC(3)	SCLOC(SCMAX)
	8F10.3			

SCLOC = average particle sizes of the active layer. This is the start of input data for sediments in the active layer. After the formation of an active layer due to deposition and coarsening, the average particle size of the active layer or deposited layer is determined. Then for that particle size the appropriate erosion rate is used. SCLOC represents the average particle sizes of the active layer for which data are available. Above 200 µm, the Roberts et al. (1998) quartz data can be used. Below that, the data is gathered from field sediments brought back to the laboratory to determine their erosion rates.

13. Comment - Critical Shear Stress for Erosion of Active Layer Bed

80
COM
80A1

COM = user specified comments for critical shear stress for erosion of active layer

14. Critical Shear Stress for Erosion of Active Layer Bed

10	20	30	
TAUCRITE(1)	TAUCRITE(2)	TAUCRITE(3)	TAUCRITE(SCMAX)
8F10.3			

TAUCRITE = critical shear stress for erosion of active layer bed at each SCLOC particle size. As the active layer particle size changes, SEDZLJ interpolates between these values to determine the critical shear stress of the active layer.





15. Comment - Erosion Rates at Each Predetermined Shear Stress

80 COM 80A1

COM = user specified comment for erosion rates at each predetermined shear stress

16. Erosion Rates at Each Predetermined Shear Stress

DO SC=1,SCMAX READ(407,'(8F10.3)') (ENRATE(SC,M),M=1,ITBM) CONTINUE

ENRATE = Erosion rates (cm/s) at each predetermined shear stress (same shear stresses

entered in 'erate.sdf' file) for each particular particle size SCLOC. SEDZLJ interpolates between these values as the active layer particle size changes.

ITBM = the number of shear stress intervals defined in 'comdeck'

17. Comment – Initial Maximum Thickness of Each Deposited Layer

80 COM 80A1

COM = user specified comment for initial maximum thickness of each deposited layer

18. Initial Maximum Thickness of Each Deposited Layer

<u>10</u> <u>DTHICKM</u> F10.3

DTHICKM = initial maximum thickness in cm of each deposited layer. Once enough material has deposited into a layer to exceed this thickness, a new layer begins filling on top of the full layer. The mass of all layers is tracked directly, so the thickness of each layer will change as a function of time, but the mass will remain constant.



19. Comment – Bulk Density

80 COM 80A1

COM = user specified comment for bulk density

20. Bulk Density

<u>10</u> <u>20</u> <u>30</u> <u>40</u> <u>DBINF</u> <u>DBSUR</u> <u>DBEXC</u> <u>DSAND</u> 4F10.3

DBINF = maximum possible bulk density,  $\rho_{\infty}$ , (g/cm<sup>3</sup>).

DBSUR = surface bulk density of initially deposited cohesive material  $(g/cm^3)$ .

DBEXC = 'c' coefficient in Eq. 6-44.

DBSAND = bulk density of pure sand at the surface as it deposits  $(g/cm^3)$ .

21. Comments - Bed Consolidation and Swelling Rates

80 COM 80A1

COM = user specified comment for bed consolidation and swelling rates

22. Bed Consolidation and Swelling Rates

10 20 DCONR DSWER 2F10.3

DCONR = consolidation rate (1/day)

DSWER = swelling rate from Eq. 6-45 (1/day)

23. Comments - Coefficients for Erosion Rates and Critical Shear Stress

80 COM 80A1

COM = user specified comment for initial maximum thickness



Coefficients for Erosion Rates and Critical Shear Stress 24.

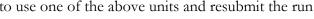
10	2	20 30	<u>40</u>
TAUSURF	ERO.	A ERON	EROM
4F10.3			
TAUSURF	=	initial critical shea	ar stress (dynes/cm <sup>2</sup> ) of a deposited cohesive layer at
		a bulk density of	DBSUR.
EROA	=	'A' coefficient in	Equation 6-46,
ERON	=	'n' and coefficient	nt in Equation 6-47,
EROM	=	'm' coefficient in	Equation 6-47,
			-

EROA, ERON, and EROM are coefficients for the determination of erosion rates in Eq. 6-46 and critical shear stresses in Eq. 6-47.

25. Number and Averaging Interval of Computational History Output Sets

10	20	30	40	50	<u>55</u>
<u>J</u> TMS	AVGE	ITRNFORM	TRANZERO	IWET	OPTAVG
I10,F10.0	),I10,F10.0,I1	0,1X,A4			_

number of times all information necessary for STSWEM will be JTMS written in "gcm\_sedtran" interval in time unit specified in OPTAVG for averaging the **AVGE** information to be written to "gcm\_sedtran" "0" - user specifies the "gcm\_sedtran" output intervals ITRNFORM = "1" - output interval will be genrated by ECOmSED based on JTMS = and NPLPFS the beginning time of "gcm\_sedtran" output TRANZERO ="0" - "gcm\_sedtran" output written for the entire grid **IWET** "1" - "gcm\_sedtran" output written for the wet grid only indicating the units of AVGE and TRANZERO. If the OPTAVG is OPTAVG not " ", "HOUR", "NDTI" or "MINU", user would be prompted to use one of the above units and resubmit the run





### Table 10-31. erate.sdf INPUT FILE

NOTE:

- 1. This file inputs all of the bed properties. Due to current model structure the first two layers are initially dummy layers and the actual sediment bed starts with layer 3. The input file still reads in data for the first two layers. It is recommended that the data for layers 1, 2, and 3 all be set equal to the initial surface interval data.
- 2. This file is required if SEDTRAN = 'INCLUDE', and SEDTYPE='SEDZLJ'
- 1. Comment Critical Shear Stress for Erosion

80 COM 80A1

COM = user specified comments for sediment transport control parameters

2. Critical Shear Stress for Erosion

10 20 30 <u>TAUTMP(1,1) TAUTMP(1,2) TAUTMP(1,3) . . . . TAUTMP(1,LAYMAX)</u> (8F10.3)

TAUTMP = critical shear stress for erosion for each layer in core in dynes/cm<sup>2</sup>.

LAYMAX = maximum number of layers specified as a parameter in *condeck*.

3. Comment -Wet Bulk Density for Each Layer

80 COM 80A1

COM = user specified comments for wet bulk density for each layer

4. Wet Bulk Density for Each Layer

10 20 30 BLKTMP(1) BLKTMP(2) BLKTMP(3) . . . . BLKTMP(LAYMAX) 8F10.3

BLKTMP = wet bulk density for each layer in the sediment bed in  $g/cm^3$ .



5. Comment - Mass Percentage of Each Size Class in Each Layer of Core

80 COM 80A1

COM = user specified comments for mass percentage of each size class in each layer of core

6. Mass Percentage of Each Size Class in Each Layer of Core

DO LL=1,LAYMAX READ (408,'(8F10.3)') (PNEW(1,LL,K),K=1,KSED) CONTINUE

PNEW = mass percentage of each size class in each layer of core. Read as a percentage not as a fraction (i.e. 100.0 = 100% of that size class).

KSED = number of particle size classes

7. Comment - Basic Shear Stresses and Erosion Rates of Core

80 COM 80A1

COM = user specified comments for basic shear stresses and erosion rates of core

9. Basic Shear Stresses and Erosion Rates of Core

DO M=1,ITBM READ (408,\*) TAULOC(M) READ(408,\*) (E0RATE(1,LL,M),LL=1,LAYMAX) CONTINUE

TAULOC = basic shear stresses for which data are available in dynes/cm<sup>2</sup>. Note

that this is the same for all cores as well as the intervals used in the

erosion rate inputs in bed.sdf.

ITBM = number of shear stress intervals defined in 'comdeck'.

E0RATE = measured erosion rates (cm/s) for each shear stress at each layer in the

core. This value is the specified erosion rate at the top of each layer.



# 10.0 Model Input Data Structure

10. Comments – Thickness of Each Layer

80 COM 80A1

COM = user specified comments for thickness of each layer

11. Thickness of Each Layer

READ(408,\*) (TSED0S(LL),LL=1,LAYMAX)

TSED0S = thickness of each layer in cm.

For multiple cores, each core is repeated and defined as above and core locations are read in through 'core\_field.sdf'.



# Table 10-32. core\_field.sdf INPUT FILE

Note: This input file is needed if SEDTRAN='INLCUDE' and SEDTYPE='SEDZLJ'

READ(94,\*) INCORE DO J=JM-1,1,-1 READ(94,2000) (CORENO(I,J),I=2,IM-1) CONTINUE FORMAT (20I3)

INCORE = number of cores used

CORENO = appropriate core number for each location in the format shown.



# Table 10-33.coh\_sed.inp INPUT FILE for SEDZLJ

Note: This input file is needed if SEDTRAN='INLCUDE' and SEDTYPE='SEDZLJ'

1. Comment – Number of Sediment Size Classes, settling velocity option for cohesives, coefficient for settling velocity equation.

 $\frac{80}{\underline{\text{COM}}}$  80A1

2. Number of Sediment Size Classes

KSED = number of sediment size classes

WSOPT = settling velocity option for cohesives. The current version only

supports "KF\_COAG" option.

WSET\_COEFF = Coefficient to be used in settling velocity equation for cohesives

3. Comment - Open Boundary Conditions for Sediment Concentrations

80 COM 80A1

4. Number of Open Boundary Grid Elements

5 NUMEBCSE I5

NUMEBCSE = total number of open boundary grid elements at which sediment

concentrations will be specified

5. Time of Observation

10 TIME F10.3



TIME = time in hours, 0.0 for initial time

6. Location of Grid Elements and Sediment Concentration Data

DO N=1,NUMEBCSE READ(IUT402,\*) II,JJ,IIC,JJC DO KK=1,KSED READ(IUT402,\*) (CBDRYSL(KK,N,K),K=1,KSL) ENDDO ENDDO

II,JJ = i and j element of grid element is specified

IIC,JJC = i and j element of connecting grid element (nearest interior non-

boundary grid elements)

CBDRYSL = sediment concentration at open boundaries

NOTE:

- 1. Sequence (II,JJ,IIC, and JJC/CBDRYSL) is repeated for each location. Total number = NUMEBSCE (total number of boundary grid elements). The sequence (TIME/CBDRYSL) is repeated for each observation. Final "TIME" must be greater than (NSTEPSxDTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEMPS x DTI)/3600 for HOT START runs. "TIME" for sediment observations need not be the same as for elevation observations in 'run data'
- 2. If HYDTYPE = 'INTERNAL', then NUMEBSCE = NUMEBC (see Data Group F, Table 8-3: Open Boundary Condition Information in 'run\_data'
- 7. Comment Sediment Concentrations at River Discharges

80 COM 80A1

8. Sediment Concentrations at River Discharges

\_\_\_\_\_5 NUMQBCSE I5

NUMQBSCE = total number of river discharges at which sediment concentrations will be specified

9. River Discharge Grid Elements



DO N=1,NUMQBCSE READ (IUT402,179)ISEQD(N),JSEQD(N),JSEQC(N),JSEQC(N) CONTINUE

ISEQD = i number of grid element discharge enters

JSEQD = j number of grid element discharge enters

ISEQC = i number of connecting exterior boundary grid element JSEQC = j number of connecting exterior boundary grid element

NOTE: Sequence ISEQD/JSEQD/ISEQD/JSEQD is repeated for each discharge location.

10. Time of Observation

10 TIME F10.3

11. Sediment Data for River Discharge

DO KK=1,KSED READ(IUT402,\*) (CDIS(KK,N),N=1,NUMQBCSE) ENDDO

CDIS = sediment concentration of river discharge in mg/l

KSED = number of sediment size classes

NOTE: 1. The sequence (TIME/CDIS) is repeated for each observation. Final "TIME" must be greater than (NSTEPSxDTI)/3600 (the duration of the run), for COLD START runs, and greater than IEND + (NSTEMPS x DTI)/3600 for HOT START runs. "TIME" for sediment observations need not be the same as for elevation observations in 'run data'

2. If HYDTYPE = 'INTERNAL', then NUMQBCSE = NUMQBC (see Data Group G, Table 8-3B: Discharge Information in 'run\_data'



# Table 10-34. timestep.inp INPUT FILE

Note: This input file is needed if DTI = 'VARI' in 'run\_data' file (i.e., user specifies a sequence of timesteps for a simulation. This feature is useful when simulating periods that include variable forcing, such as river flow or wind conditions, which result in temporal variations of minimum timesteps.

### 1. Comment

80 COM 80A1

# 2. Variable Timesteps

10	20	30
NUM	TNEXT	DTI

NUM = sequential number. This value is not used by ECOMSEDZLJ TNEXT = Ending time (days) for use of specified timestep (DTI)

DTI = Timestep in seconds

NOTE: 1. There is no limit on the number of pairs of TNEXT and DTI.

- 2. TNEXT must increase monotonically and be an integer multiple of DTI
- 3. The last value of TNEXT must be greater than or equal to the ending time of the simulation.
- 4. Sequential values of DTI should change gradually to ensure stable model results. It is recommended that sequential values of DTI change by no more than 50 percent.



# 11.0 Model Output Data Structure

# Table 11-1. Summary of Model Generated Output Files

Tubic 11-1. Guillin	ary or it	iodel delicitica output i lies
<u>File</u>		
A. gcmprt	-	this file is a formatted output file. It contains all input information as well as many model computed values.
B. gcmplt	-	this file is an unformatted output file. It contains the computed results for all grid elements at the times and for the intervals specified in the file "run_data". The contents of this file are described in detail in this section.
C. gcmtsr	-	this file is an unformatted output file. It contains the computed values of elevation, current, temperature, salinity, conservative tracer and fluxes for grid elements specified in the "run_data" file, as well as run-time global integrals of various parameters. The contents of this file are described in detail in this section.
D. part_location	-	this file is a formatted output file. It contains the computed locations of particles during a particle tracking simulation. This file is generated if PARTICLE = "INCLUDE" in "run_data." The contents of this file are described in detail in this section.
E. gcm_tran	-	this file is an unformatted output file. It contains computed results of surface elevations, volume transports and dispersions as a time history. It is to be used as input to a water quality model. The contents of this file are described in detail in this section.
F. gcm_geom	-	this file is an unformatted output file. It contains grid segmentation information. It is to be used as input to a water quality model. The contents of this file are described in detail in this section.
G. startup	-	this file is an unformatted output file. It contains all the information for the hydrodynamic model run which will become the initial conditions for the "HOT START" runs. The user should move or copy the "startup" file to "restart" before making the
H. cseds.out	-	next "HOT START" run. this file is an unformatted output file. It contains hourly water column solids concentrations. The contents of this file are described in detail in this section.
I. cseds_pval.out	-	this file is an unformatted output file. It contains hourly size fractions of water column solids. The contents of this file are described in detail in this section.
J. dbl.out	-	this file is an unformatted output file. It contains hourly bed load depositional flux values. The contents of this file are described in detail in this section.
K.dbl2ac.out	-	this file is an unformatted output file. It contains hourly values of the cumulative bed load depositional flux values. The contents of this file are described in detail in this section.
L. ddd.out	-	this file is an unformatted output file. It contains hourly water column solids depositional flux values. The contents of this file are described in detail in this section.
M.ddd2ac.out	-	this file is an unformatted output file. It contains hourly values of the cumulative water column solids depositional flux values. The contents of this file are described in detail in this section.



N. ee.out

this file is an unformatted output file. It contains hourly sediment erosional flux values.

The contents of this file are described in detail in this section.

### 11.0 Model Output Data Structure

O. ee2ac.out - this file is an unformatted output file. It contains hourly values of the cumulative sediment erosional flux values. The contents of this file are described in detail in this section.

P. gcmsedplt - this file is an unformatted output file. It contains sediment transport model output for HydroQual's proprietary model output viewer

Q. gcm\_sedtran - this file is an unformatted output file. It contains sediment transport model output information for linkage to the organic carbon fate model (STSWEM). The contents of this file are described in detail in this section.

R. psus.out - this file is an unformatted output file. It contains hourly fractions of resuspension to the water column (fraction to bedload is 1 - PSUS). The contents of this file are described in detail in this section.

S. qsed.out - this file is an unformatted output file. It contains resuspension flux to the water column printed at hourly intervals. The contents of this file are described in detail in this section.

T. qbsed.out - this file is an unformatted output file. It contains resuspension flux to bed load printed at hourly intervals. The contents of this file are described in detail in this section.

U. sedtec2d.dat - this file is a formatted output file. It contains two dimensional sediment transport output, including bed elevation change, grain shear stress, bed load fluxes and vertically averaged water column solids concentration printed at hourly intervals.

V. sedtec3d.dat - this file is a formatted output file. It contains three dimensional sediment transport output, water column solids concentration and water velocity printed at hourly intervals.



### Table 11-2. gcmplt OUTPUT FILE (UNFORMATTED)

```
READ(20) IM,JM,KB
          READ(20) EBCM, QBCM, NCHEMLAY
          READ(20) DTI,GRAV,UMOL,TOR, TRACER, SEDTRAN, CHEMTRAN
          READ(20) NUMEBC
          READ(20) (IETA(I),JETA(I),ICON(I),JCON(I),I=1,NUMEBC)
          READ(20) NUMQBC
          READ(20) (IQC(I),JQC(I),I=1,NUMQBC)
          READ(20) H
          READ(20) H1
          READ(20) H2
          READ(20) ANG
          READ(20) DUM
          READ(20) DVM
          READ(20) FSM
С
          DO 1000 JHIST=1,JHM
            READ(20) TMIDDLE
            READ(20) ARCET
            IF(TOR.EQ.'BAROTROPIC') THEN
              READ(20) ((ARCU (I,J,1),I=1,IM),J=1,JM)
              READ(20) ((ARCV (I,J,1),I=1,IM),J=1,JM)
              READ(20) ((ARCUX(I,J,1),I=1,IM),J=1,JM)
              READ(20) ((ARCVX(I,J,1),I=1,IM),J=1,JM)
            IF (TRACER.EQ.'INCLUDE') READ (20) ((ARCC(I,J,1),I=1,IM),J=1,JM)
            IF (SEDTRAN.EQ.'INCLUDE') THEN
              READ (20) ((ARCSED1(I,J,1),I=1,IM),J=1,JM)
              READ (20) ((ARCSED2(I,J,1),I=1,IM),J=1,JM)
              READ (20) ((ARCTHIK(I,J),I=1,IM),J=1,JM)
              ENDIF
            IF (CHEMTRAN.EQ.'INCLUDE') THEN
              READ (20) ((ARCCHEM1(I,J,1),I=1,IM),J=1,JM)
              READ (20) ((ARCCHEM2(I,J,1),I=1,IM),J=1,JM)
              READ (20) ((ARCPBED(N,I,J),I=1,IM),J=1,JM),N=1,NCHEMLAY)
              ENDIF
          ELSE
              READ(20) Z
              READ(20) ZZ
              READ(20) DZ
              READ(20) ARCU
              READ(20) ARCV
              READ(20) ARCUX
              READ(20) ARCVX
              READ(20) ARCT
              READ(20) ARCS
              READ(20) ARCW
              READ(20) ARCKH, ARCKM
            IF (TRACER.EQ.'INCLUDE') READ(20) ARCC
            IF (SEDTRAN.EQ.'INCLUDE') THEN
              READ (20) ARCSED1
              READ (20) ARCSED2
              READ (20) ARCTHIK
              READ (20) ARCTAU
              ENDIF
            IF (CHEMTRAN.EQ.'INCLUDE') THEN
```



READ (20) ARCCHEM1 READ (20) ARCCHEM2

READ (20) ((ARCPBED(N,I,J),I=1,IM),J=1,JM),N=1,NCHEMLAY)

ENDIF 1000 CONTINUE

Unit 20 "gcmplt" IM total number of grid elements in the  $\xi_1$  direction total number of grid elements in the  $\xi_2$  direction JM KΒ number of sigma levels = **EBCM** maximum number of elevation boundary grid elements **QBCM** maximum number of discharge boundary grid elements DTI time step of the internal mode (sec) **GRAV** gravitational acceleration (m<sup>2</sup>/sec) constant or background mixing (m<sup>2</sup>/sec) **UMOL** type of run ("BAROTROPIC"/"PROGNOSTIC"/"DIAGNOSTIC") TOR **NCHEMLAY** number of layers in sediment-bound tracer bed model **TRACER** control parameter for dissolved tracer transport control parameter for sediment transport **SEDTRAN** = **CHEMTRAN** control parameter for sediment-bound tracer transport total number of elevation boundary grid elements NUMEBC **IETA** i number of grid element where elevation is specified **JETA** j number of grid element where elevation is specified **ICON** i number of connecting grid element (nearest interior non-boundary grid element) **JCON** i number of connecting grid element (nearest interior non-boundary grid element) **NUMQBC** total number of discharge boundary grid elements **IQC** i number of grid element where discharge enters/leaves JQC i number of grid element where discharge enters/leaves average depth of grid element (m) Η H1 distance in the  $\xi_1$  direction at the center of the grid (m) distance in the  $\xi_2$  direction at the center of the grid (m) H2 **ANG** angle between east and the ξ<sub>1</sub> direction measured in a counter-clockwise direction = (dea) DUM land/water mask at the U interface of the grid element DVM land/water mask at the V interface of the grid element **FSM** land/water mask at the center of the grid element **TMIDDLE** time at the middle of the time interval (days) free surface elevation of the grid element (m) **ARCET** depth of the interface between sigma levels 0.0 at the surface -1.0 at the bottom ZZ intermediate depth between sigma levels DΖ thickness of the sigma level Z(K) - Z(K+1)**ARCU** velocity component in the  $\xi_1$  direction (m/sec) velocity component in the  $\xi_2$  direction (m/sec) transport component in the  $\xi_1$  direction (m²/sec) **ARCV** \_ **ARCUX** = **ARCVX** transport component in the  $\xi_2$  direction (m<sup>2</sup>/sec) = temperature of the grid element (°C) **ARCT** = salinity of the grid element (psu) **ARCS ARCW** vertical velocity (m/sec) vertical eddy diffusivity (m<sup>2</sup>/sec) **ARCKH ARCKM** vertical eddy viscosity (m<sup>2</sup>/sec) **ARCC** conservative tracer concentration (only included if TRACER = "INCLUDE")



# 11.0 Model Output Data Structure

ARCSED1 cohesive sediment concentration (mg/l) (only included if SEDTRAN = "INCLUDE") non-cohesive sediment concentration (mg/l) (only included if SEDTRAN = "INCLUDE") ARCSED2 sediment bed elevation change (cm) **ARCTHIK** (only included if SEDTRAN = "INCLUDE") bottom shear stress for use in sediment transport (dynes/cm²) **ARCTAU** cohesive sediment-bound tracer concentration (µg/l) ARCCHEM1 (only included if CHEMTRAN = "INCLUDE") ARCCHEM2 non-cohesive sediment-bound tracer concentration (µg/l) (only included if CHEMTRAN = "INCLUDE") sediment bed concentration of sediment-bound tracer (ppm) **ARCPBED** (only included if CHEMTRAN = "INCLUDE")



### Table 11-3. gcmtsr OUTPUT FILE (UNFORMATTED)

```
READ(30) TOR, TRACER, SEDTRAN, CHEMTRAN
          READ(30) KBM1, NCHEMLAY
          READ(30) EPTS
          READ(30) (INXIE(N),INXJE(N),N=1,EPTS)
          READ(30) VPTS
          READ(30) (INXIV(N),INXJV(N),N=1,VPTS)
          READ(30) (ANG (INXIV(N),INXJV(N)),N=1,VPTS)
          READ(30) FPTS
          READ(30) (ISFLX(N), JSFLX(N), DIRFLX(N), NFLXE(N), N=1, FPTS)
С
          DO 1000 I=1,ID
            READ(30) TMIDDLE
            READ(30) (ESAVE(N), N=1, EPTS)
          IF(TOR.EQ.'BAROTROPIC') THEN
              READ(30) (UZSAVE(N,1), VZSAVE(N,1), N=1, VPTS)
            IF (TRACER.EQ.'INCLUDE') READ (30) (C1ZSAVE(N,1),N=1,VPTS)
            IF (SEDTRAN.EQ.'INCLUDE') THEN
              READ (30) (C1SAVE(N,1),C2SAVE(N,1),N=1,VPTS)
              READ (30) (THSAVE(N), N=1, VPTS)
              READ(30) (TAUSAVE(N,1), N-1, VPTS)
              ENDIF
            IF (CHEMTRAN.EQ.'INCLUDE') THEN
              READ (30) (P1SAVE(N,1),P2SAVE(N,1),N=1,VPTS)
              READ (30) ((PBEDSAVE(N,LL),N=1,VPTS),LL=1,NCHEMLAY)
              READ(30) (CCFLUX(N,1),N=1,FPTS)
              READ(30) ESUM, TKE, APE
            ELSE
              READ(30) (DZSAVE(N), N=1, VPTS)
              READ(30) ((UZSAVE(N,K), VZSAVE(N,K), SZSAVE(N,K), TZSAVE(N,K),
                        N=1,VPTS), K=1,KBM1), (((KHZSAVE(N,K), KMZSAVE(N,K), N = VPTS, K = 1, KBM1)
            IF (TRACER.EQ.'INCLUDE') READ (30) ((C1ZSAVE(N,K),N=1,VPTS),
               K=1,KBM1)
            IF (SEDTRAN.EQ.'INCLUDE') THEN
              READ (30) ((C1SAVE(N,K),C2SAVE(N,K),N=1,VPTS),K=1,KBM1)
              READ (30) (THSAVE(N), N=1, VPTS)
              READ (30) (TAUSAVE(N,KB),-1,VPTS)
              ENDIF
            IF (CHEMTRAN.EQ.'INCLUDE') THEN
              READ (30) ((P1SAVE(N,K),P2SAVE(N,K),N=1,VPTS),K=1,KBM1)
              READ (30) ((PBEDSAVE(N,LL),N=1,VPTS),LL=1,NCHEMLAY)
            READ(30) ((CCFLUX(N,K),N=1,FPTS),K=1,KBM1)
              READ(30) VSTOR, EM, APEC, TSUM, SSUM
```

### 1000 CONTINUE

Unit 30 = "gcmtsr"

TOR = type of run ("BAROTROPIC"/"PROGNOSTIC"/"DIAGNOSTIC")

NCHEMLAY = number of layers in sediment-bound tracer bed model TRACER = control parameter for dissolved tracer transport SEDTRAN = control parameter for sediment transport

CHEMTRAN = control parameter for sediment-bound tracer transport

KBM1 = number of sigma layers (KB-1)

EPTS = number of grid elements with elevation time series



INXIE = i number of user specified grid element INXJE = j number of user specified grid element

VPTS = number of grid elements with current time series

INXIV = i number of user specified grid element INXJV = j number of user specified grid element

ANG = angle in degrees between east and ξ, direction measured in a counter-clockwise

direction

FPTS = number of user specified grid elements with cross sectional flux time series
ISFLX = i number of user specified grid element in which cross section begins

JSFLX = j number of user specified grid element in which cross section begins

DIRFLX = direction of the cross section

NFLXE

C1SAVE

= "IDIR" - cross section in the  $\xi_1$  direction = "JDIR" - cross section in the  $\xi_2$  direction number of grid elements in the cross section = time at the middle of the time interval (days)

TMIDDLE = time at the middle of the time interval (days)
ESAVE = surface elevation of the user specified grid element (m)

DZSAVE = total depth of the user specified grid element (m)

= bottom topography + elevation

UZSAVE = U velocity averaged at the center of the user specified grid element (m/sec)
VZSAVE = V velocity averaged at the center of the user specified grid element (m/sec)

SZSAVE = salinity of the user specified grid element (psu)
TZSAVE = temperature of the user specified grid element (°C)

KHZSAVE = vertical eddy diffusivity (m²/sec) KMZSAVE = vertical eddy viscosity (m²/sec)

CCFLUX = mass transport averaged at the center of the user specified grid element (m<sup>3</sup>/sec)

ESUM = average surface elevation in the modeling domain (m)

TKE = volume averaged total kinetic energy (joule)

APE = volume averaged available potential energy (joule)

VSTOR = volume storage (m³) EM = excess mass (kg)

APEC = excess volume averaged available potential energy (joule)
SSUM = volume averaged salinity in the modeling domain (psu)
TSUM = volume averaged temperature in the modeling domain (°C)

C1ZSAVE = conservative tracer concentration

(only included if TRACER = "INCLUDE")
cohesive sediment concentration (mg/l)
(only included if SEDTRAN = "INCLUDE")

C2SAVE = non-cohesive sediment concentration (mg/l) (only included if SEDTRAN = "INCLUDE")

THSAVE = sediment bed elevation change (cm)
(only included if SEDTRAN = "INCLUDE")

TAUSAVE = bottom shear stress for use in sediment transport (dynes/cm²)

P1SAVE = cohesive sediment-bound tracer concentration (µg/l)

(only included if CHEMTRAN = "INCLUDE")

P2SAVE = non-cohesive sediment-bound tracer concentration (µg/l)

(only included if CHEMTRAN = "INCLUDE")

PBEDSAVE = sediment bed concentration of sediment-bound tracer (ppm)

(only included if CHEMTRAN = "INCLUDE")



# Table 11-4. part\_location OUTPUT FILE (FORMATTED)

Unit 40 = "part\_location

NSOURCE = number of particle sources

NGRADELOOP = number of releases

NPART = number of particles per release

TIME = time (days) when the locations of released particles are recorded

XOUTP = particle location in x-direction (East) (m)
YOUTP = particle location in y-direction (North) (m)
ZOUTP = particle location in z-direction (Up) (m)



# Table 11-5. gcm\_tran OUTPUT FILE (UNFORMATTED)

```
DO 1000 JTRAC=1,JTM
READ(10) TMIDDLE
READ(10) (((ULPF(I,J,K),I=1,IM),J=1,JM),K=1,KBM1)
READ(10) (((VLPF(I,J,K),I=1,IM),J=1,JM),K=1,KBM1)
READ(10) WLPF
READ(10) (((AAMAX(I,J,K),I=1,IM),J=1,JM),K=1,KBM1)
READ(10) (((AAMAY(I,J,K),I=1,IM),J=1,JM),K=1,KBM1)
READ(10) KHLPF
READ(10) KMLPF
READ(10) ES
READ(10) ES
READ(10) ED
READ(10) (((SLPF(I,J,K),I=1,IM),J=1,JM),K=1,KBM1)
READ(10) (((TLPF(I,J,K),I=1,IM),J=1,JM),K=1,KBM1)
READ(10) (((TLPF(I,J,K),I=1,IM),J=1,JM),K=1,KBM1)
```

Unit 10	= "g	jcm_tran"
TMIDDLE	=	time at the middle of the time averaging interval (days)
ULPF	=	low pass filtered volume flow rate in the ξ <sub>1</sub> direction (m3/sec)
VLPF	=	low pass filtered volume flow rate in the $\xi$ , direction (m <sup>3</sup> /sec)
WLPF	=	low pass filtered vertical volume flow rate (m³/sec)
AAMAX	=	low pass filtered horizontal eddy viscosity in $\xi_1$ direction (m <sup>2</sup> /sec)
AAMAY	=	low pass filtered horizontal eddy viscosity in $\xi_2$ direction (m <sup>2</sup> /sec)
KHLPF	=	low pass filtered vertical eddy diffusivity (m²/sec)
KMLPF	=	low pass filtered vertical eddy viscosity (m²/sec)
ES	=	initial surface elevation (m)
ED	=	time rate of change of elevation (m/sec)
SLPF	=	low pass filtered salinity (psu)
TLPF	=	low pass filtered temperature (°C)



# Table 11-6. gcm\_geom OUTPUT FILE (UNFORMATTED)

READ(10) DZ,DZZ READ(10) H,H1,H2,TPS READ(10) ANG, NU

Unit 10	= "gcm_geom"		
DZ	=	thickness of the sigma level	
DZZ	=	average depth of the grid element (m)	
H1	=	distance in the $\xi_1$ direction at the center of the grid (m)	
H2	=	distance in the $\xi_{i}$ direction at the center of the grid (m)	
TPS	=	land/water mask at the center of the grid element	
ANG	=	angle between east and the $\xi_1$ direction measured in a counter- clockwise direction (deg)	
NU	=	coefficient in time filter (non-dimensional)	



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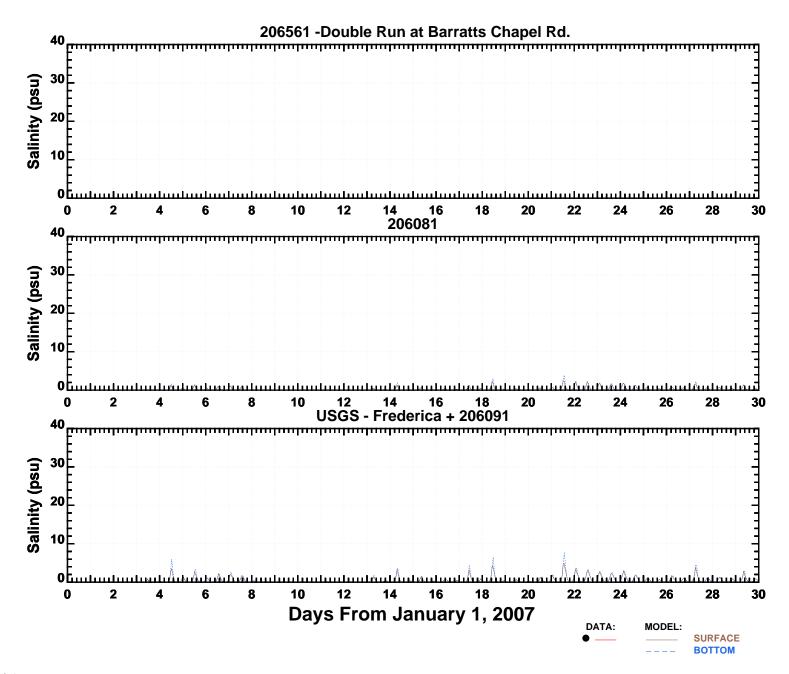
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# **APPENDIX 4**

# HYDRODYNAMIC MODEL SALINTY & TEMPERATURE CALIBRATION/VALIDATION FIGURES

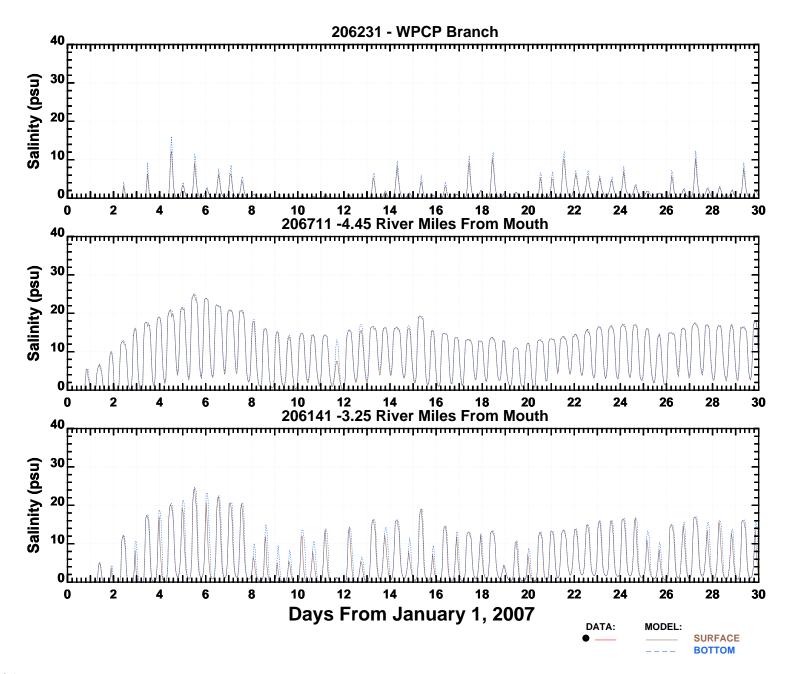


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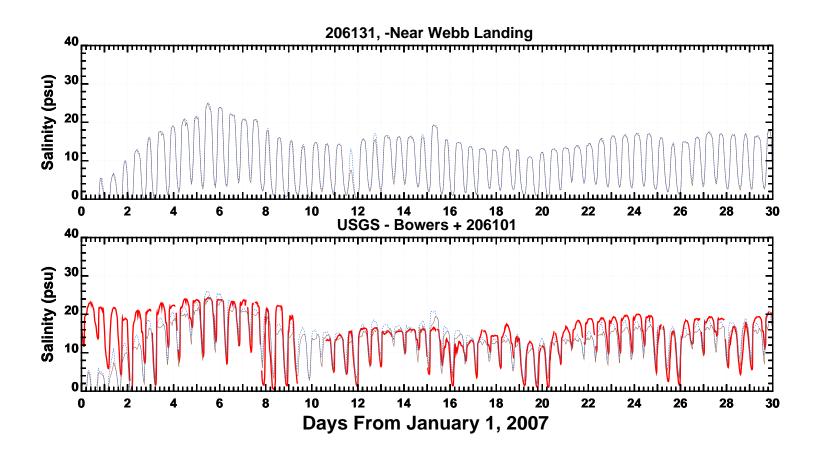


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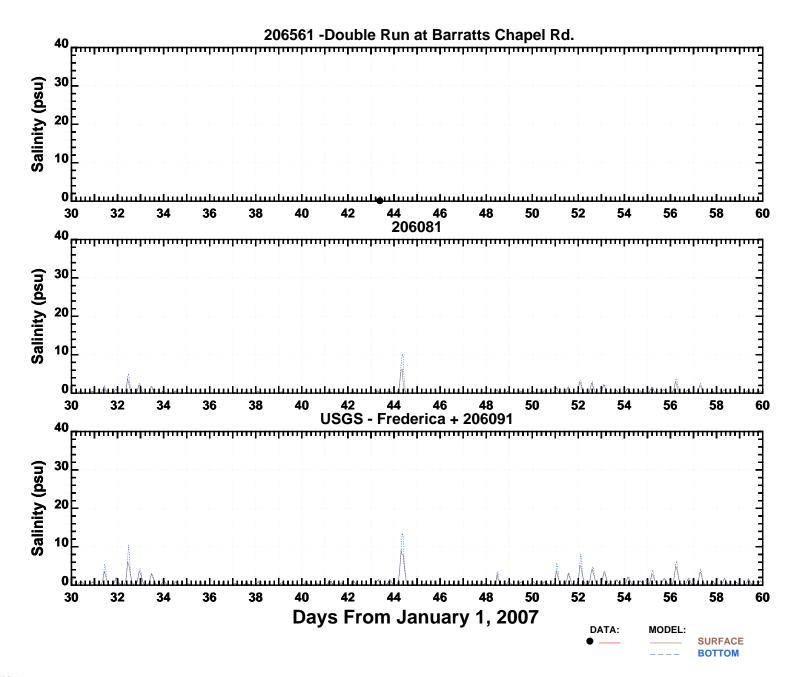
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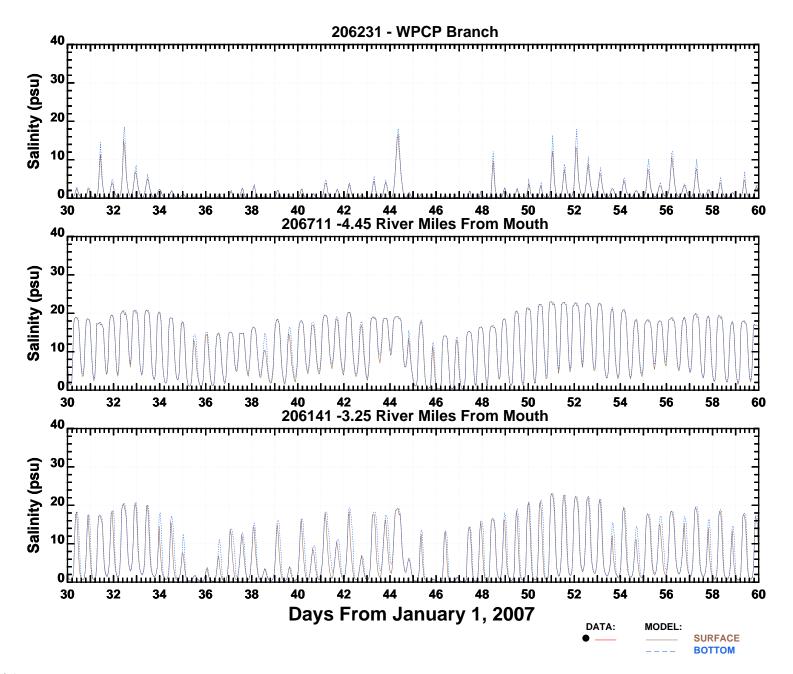


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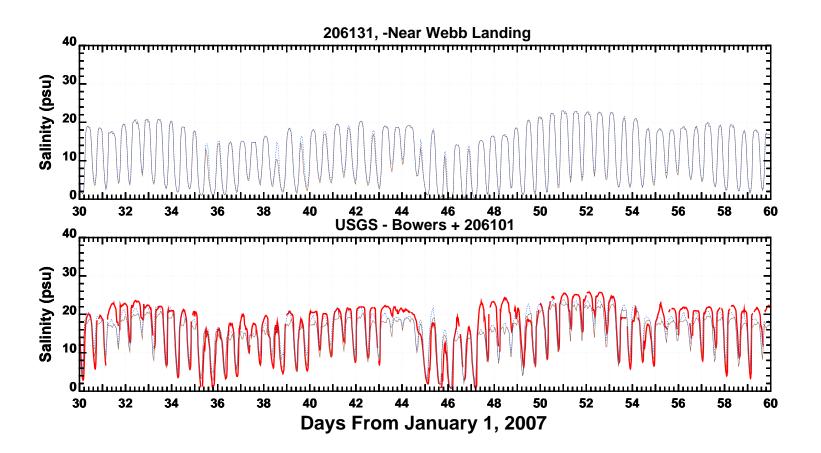


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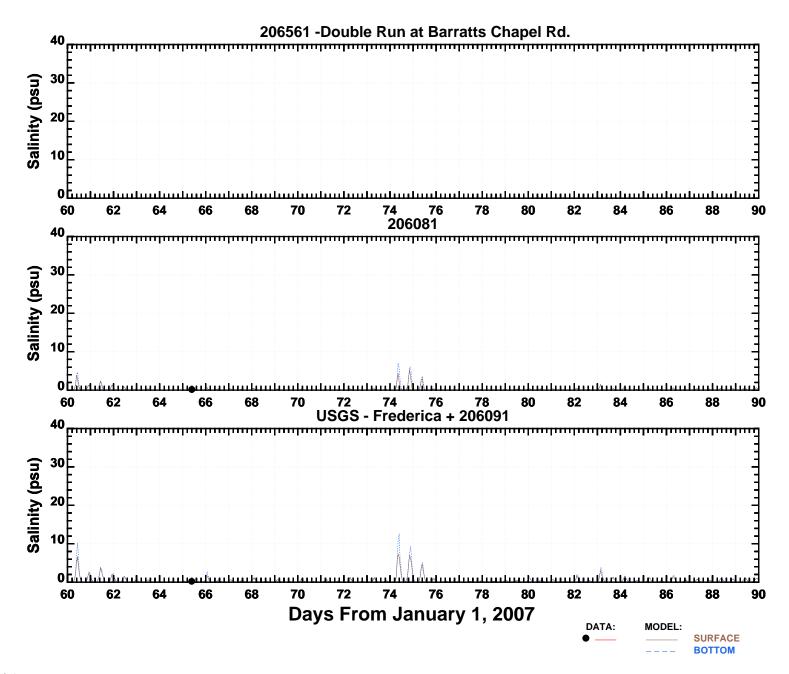
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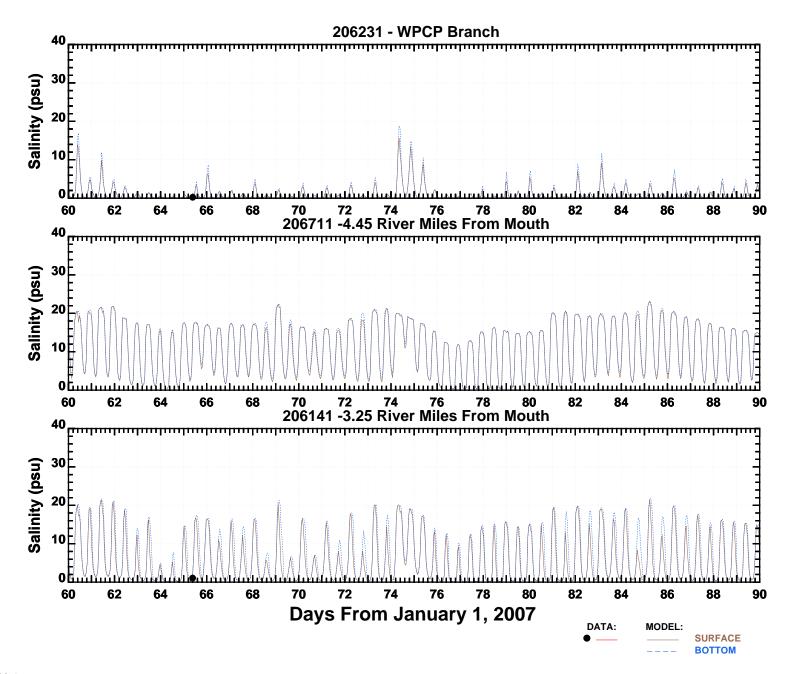


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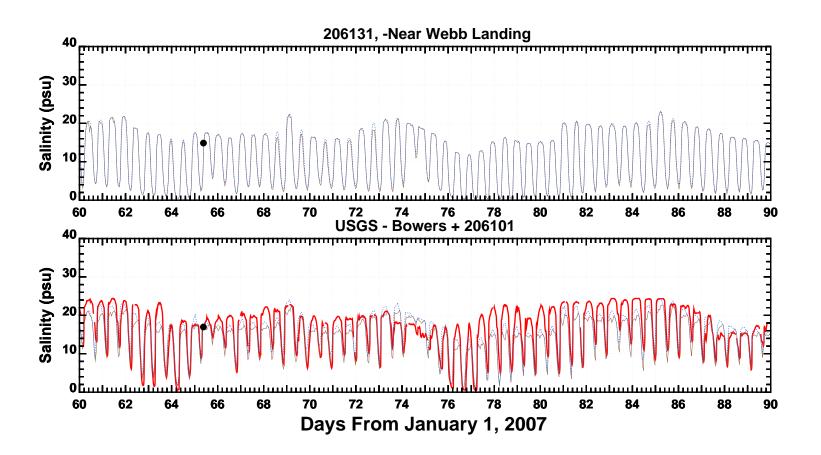


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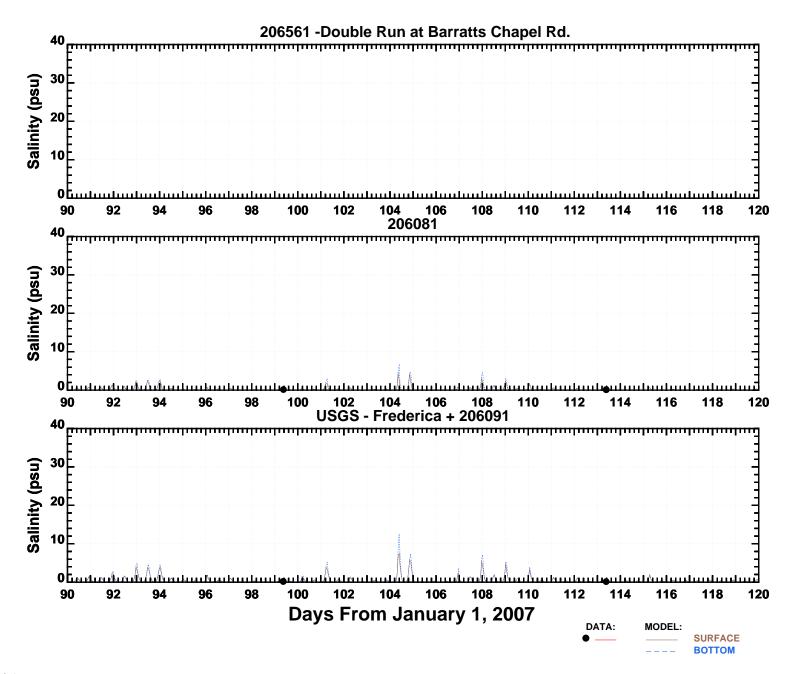
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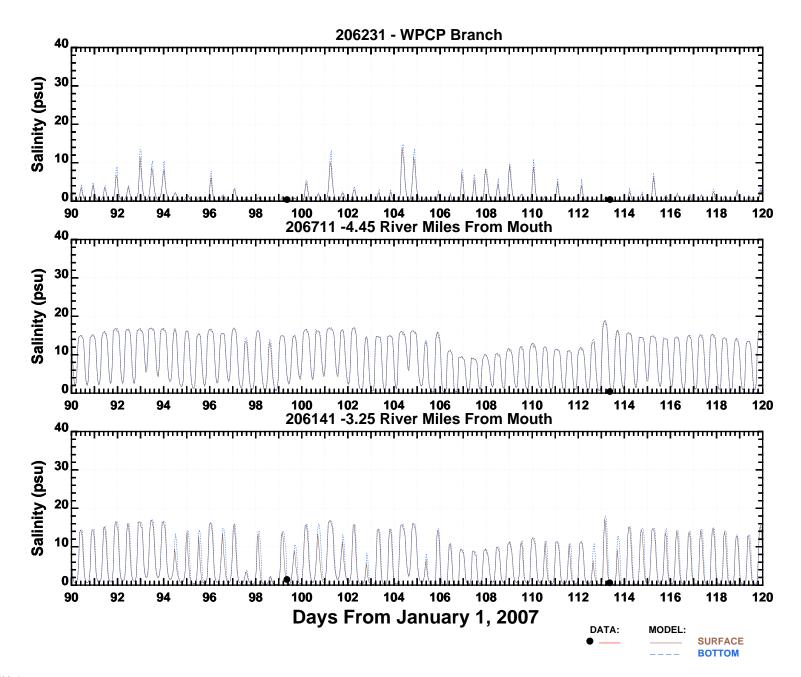


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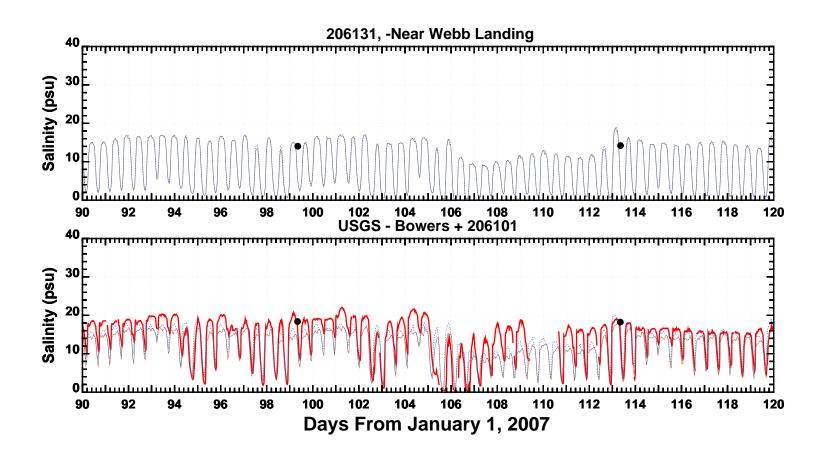


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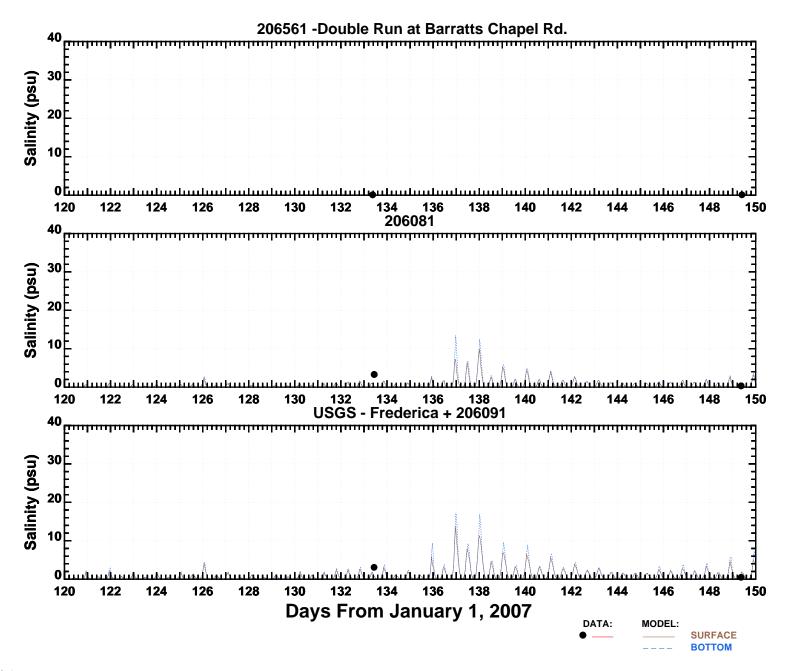


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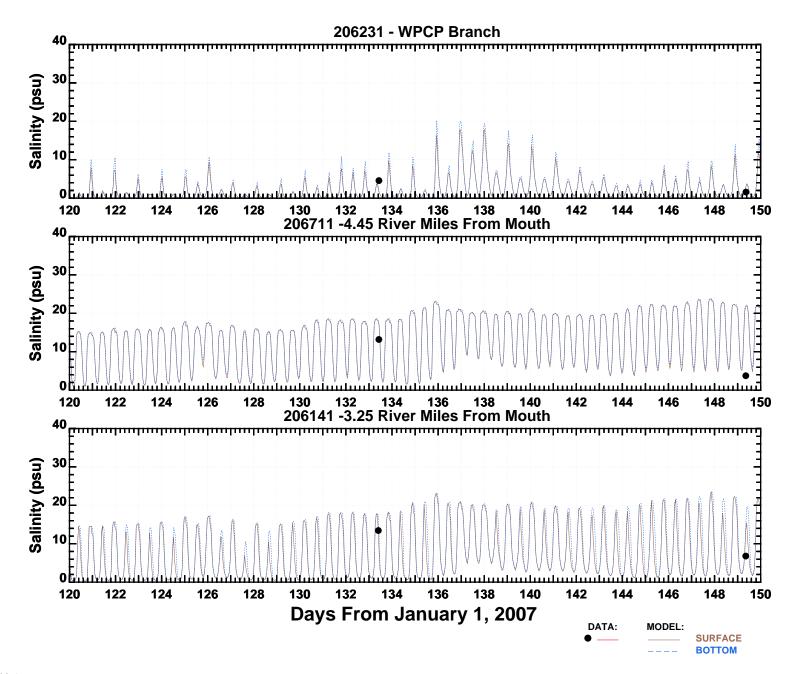


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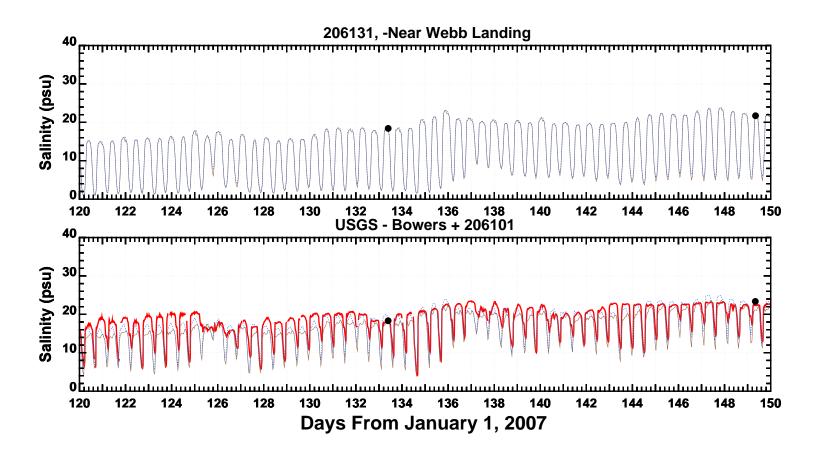


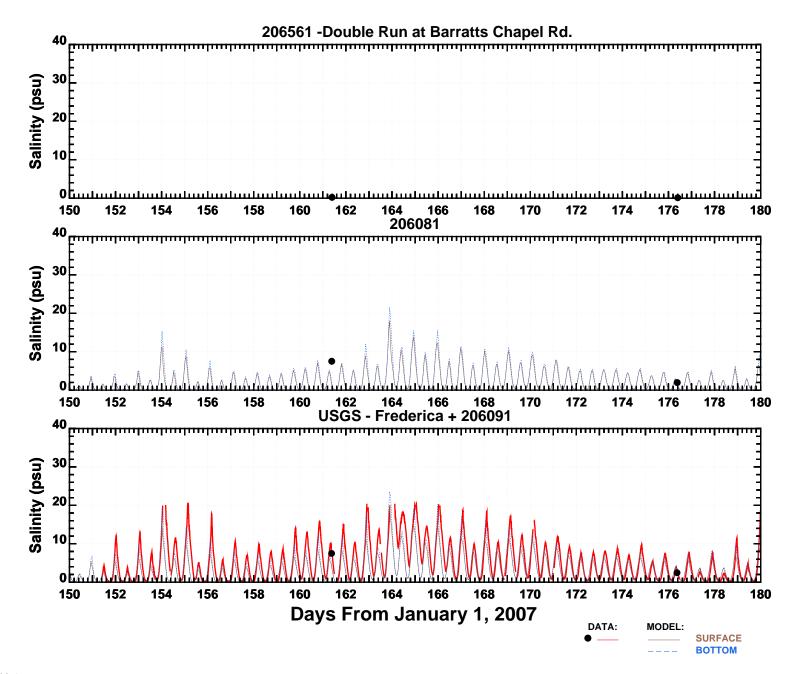
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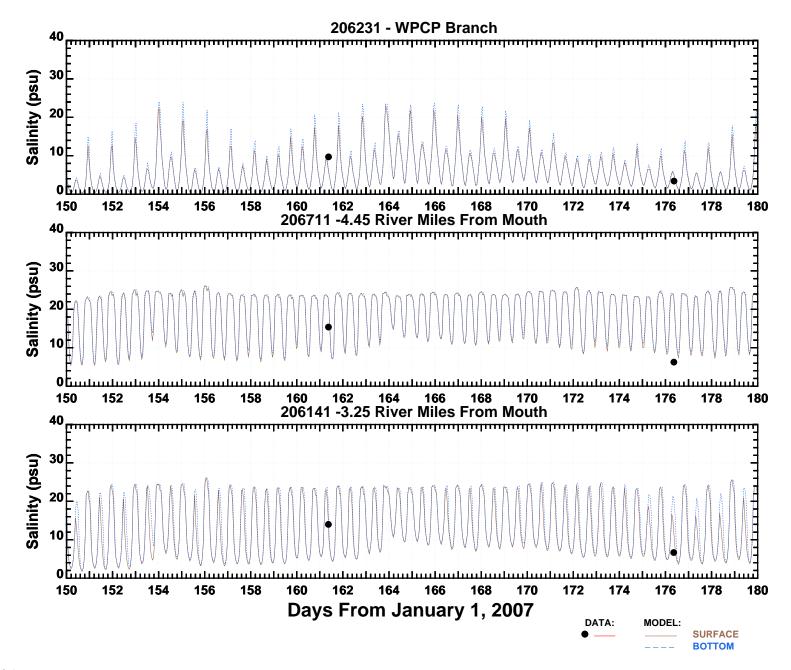


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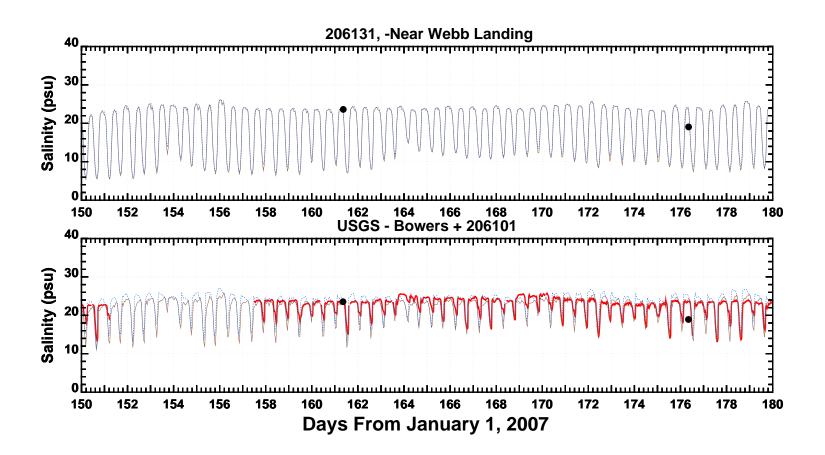


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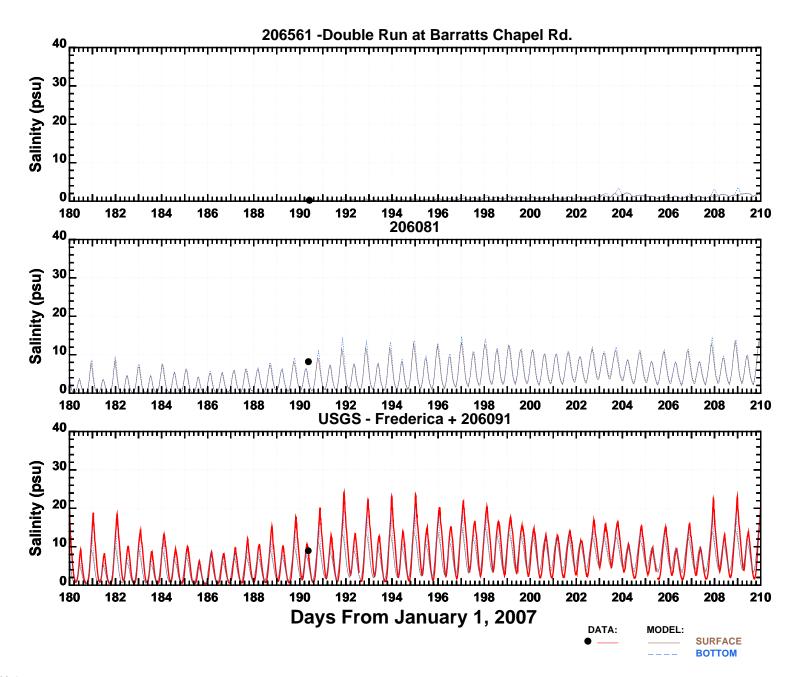


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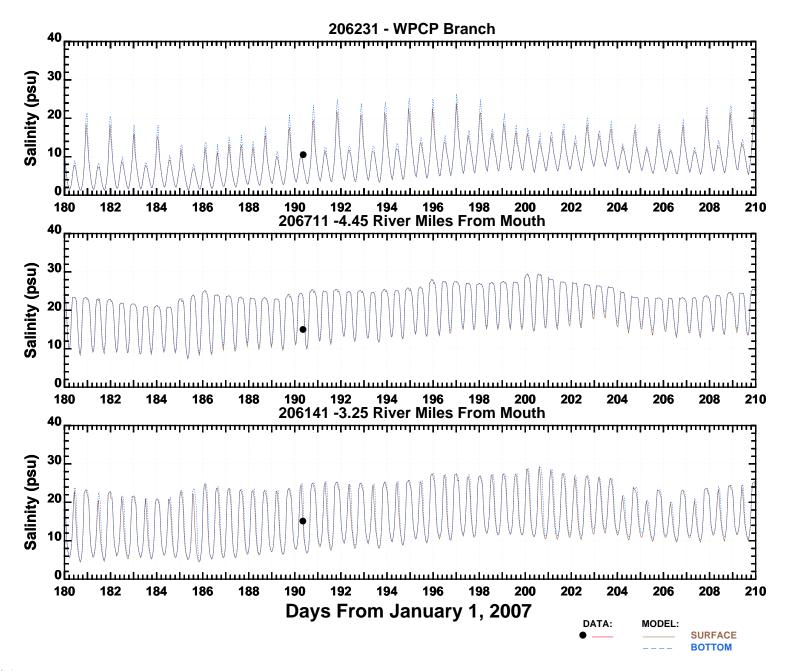
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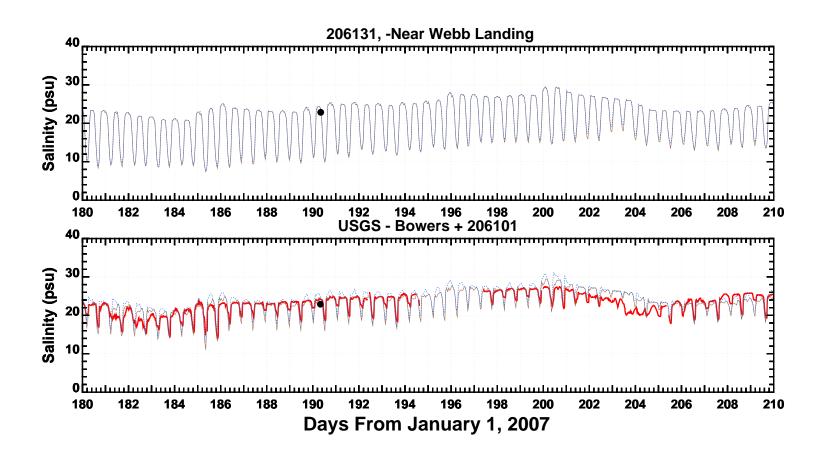
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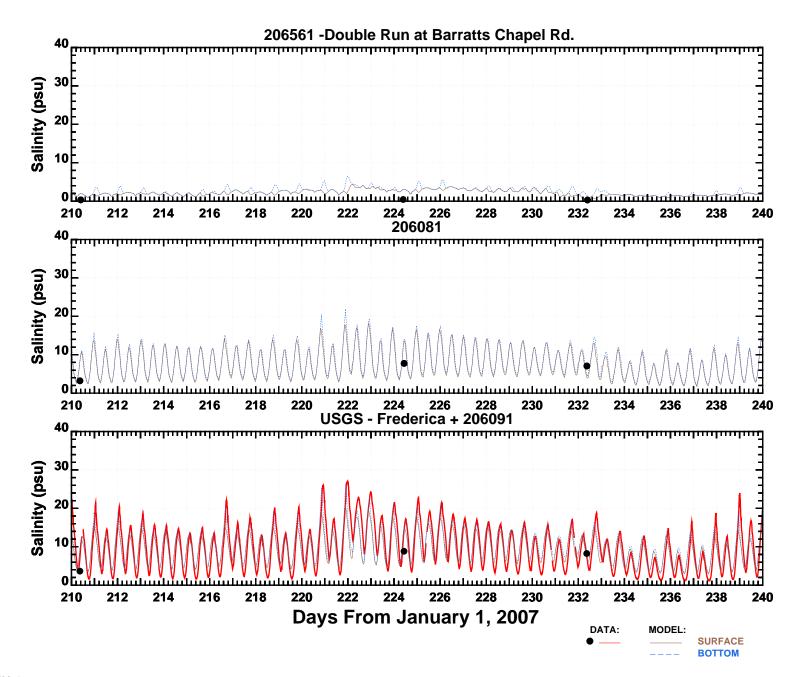


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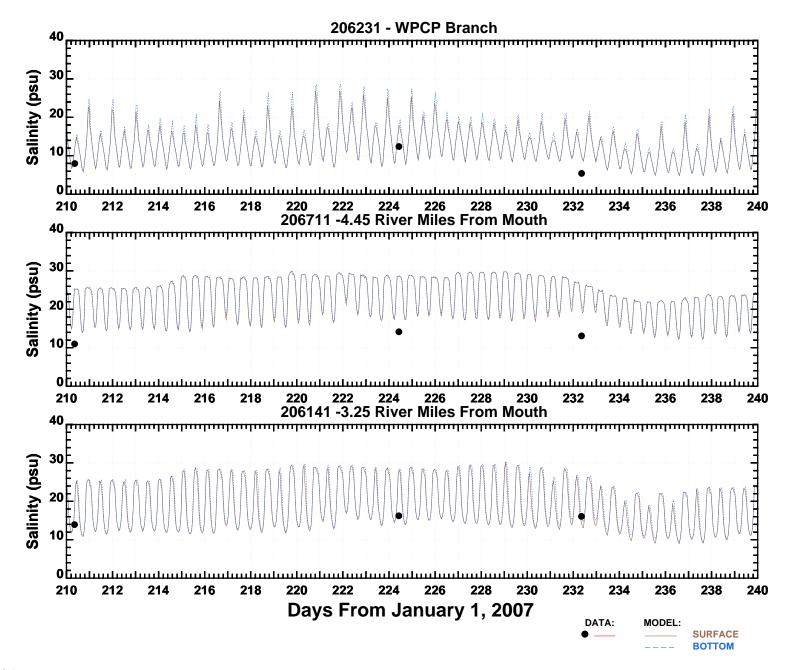
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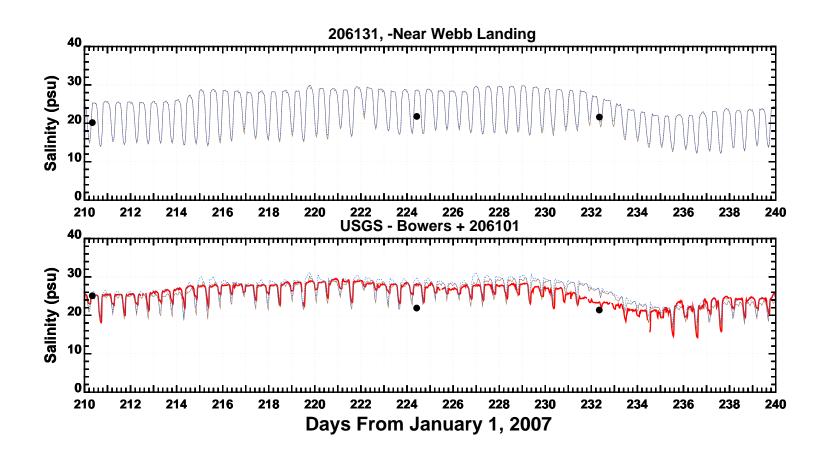
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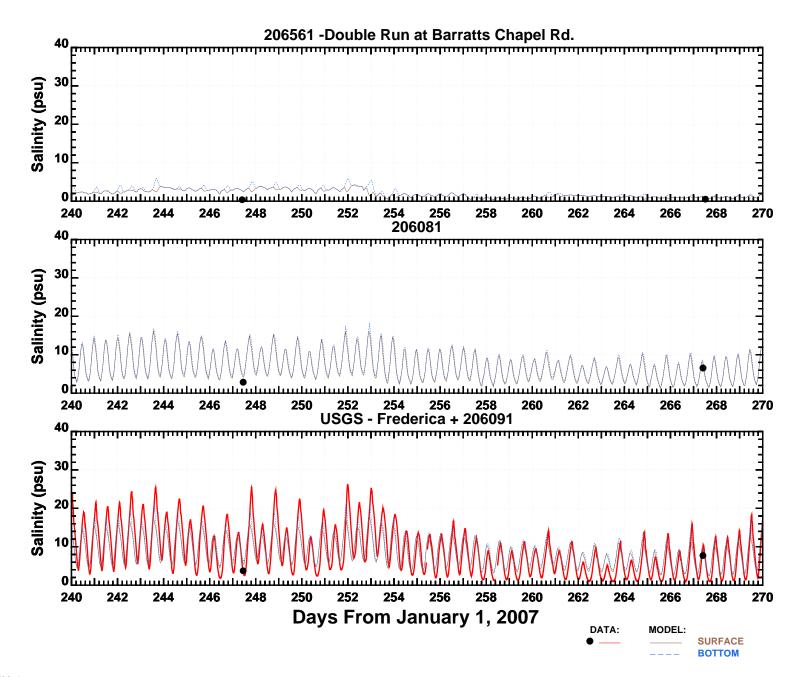


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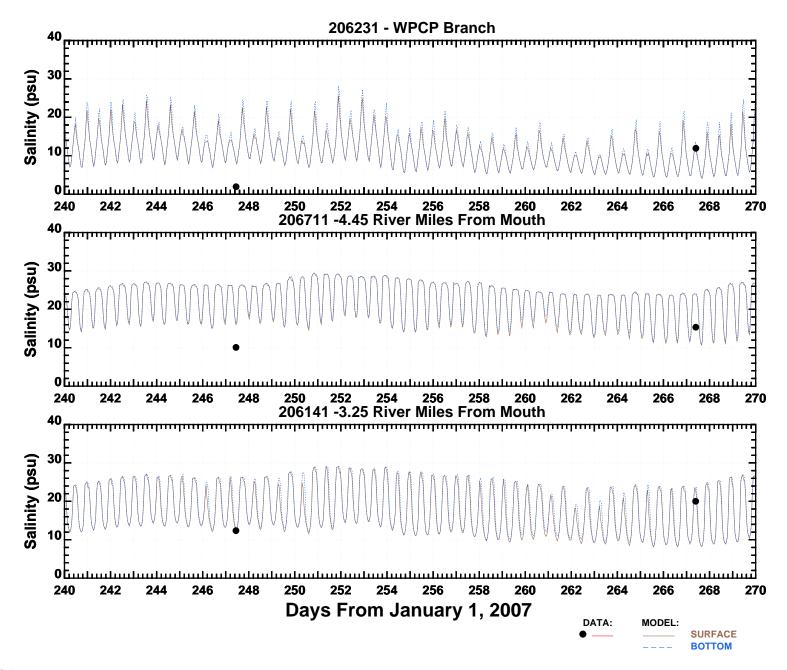


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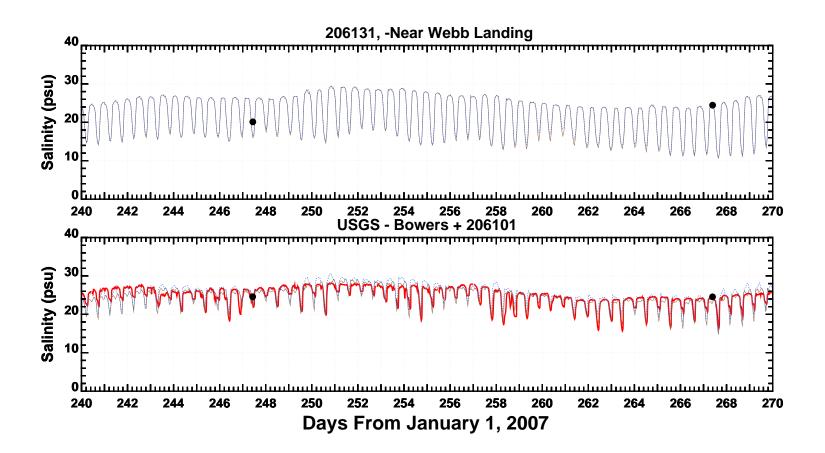




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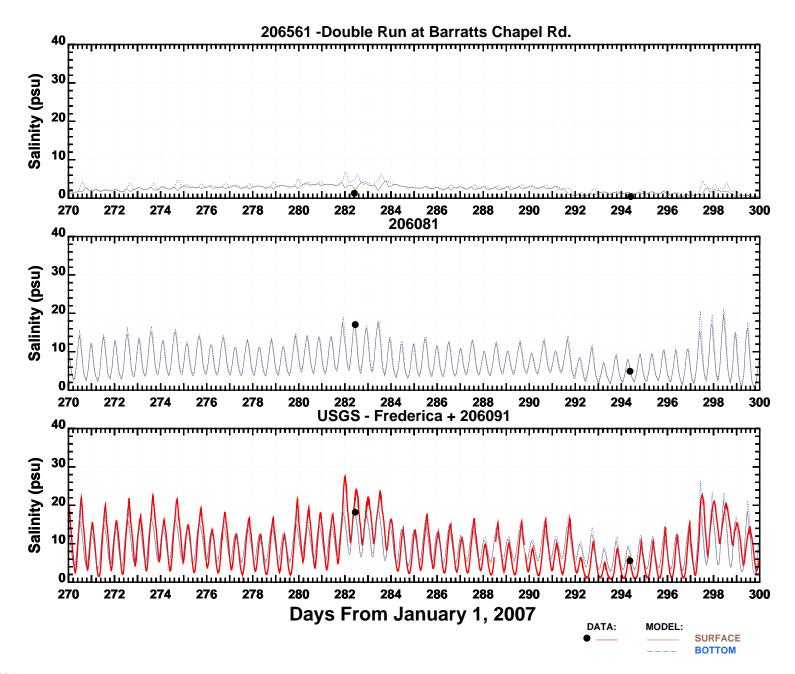


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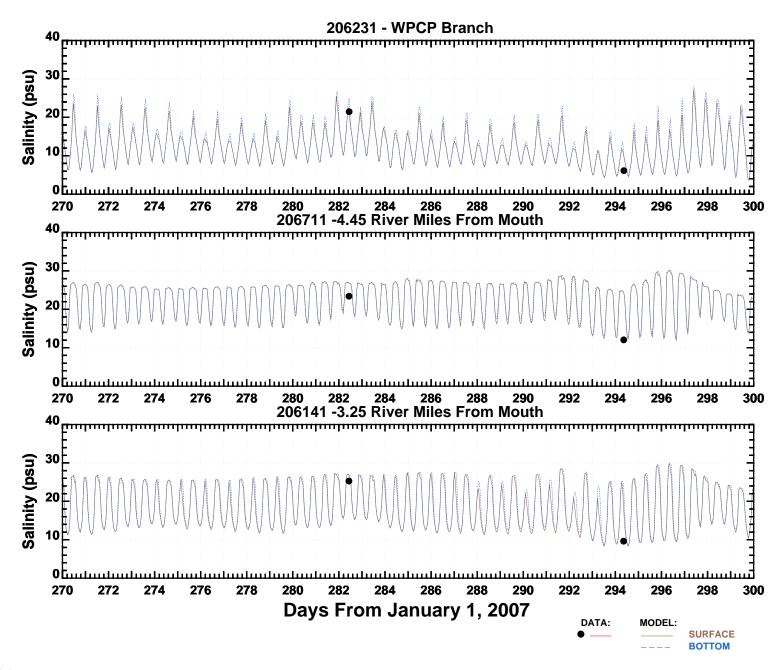
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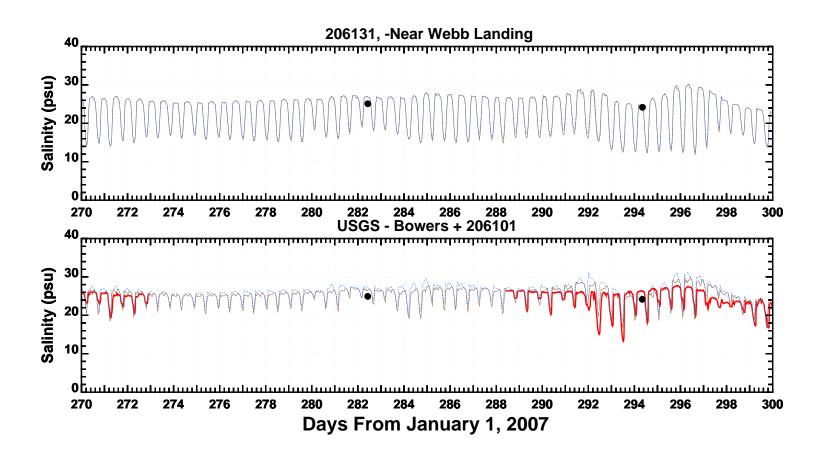
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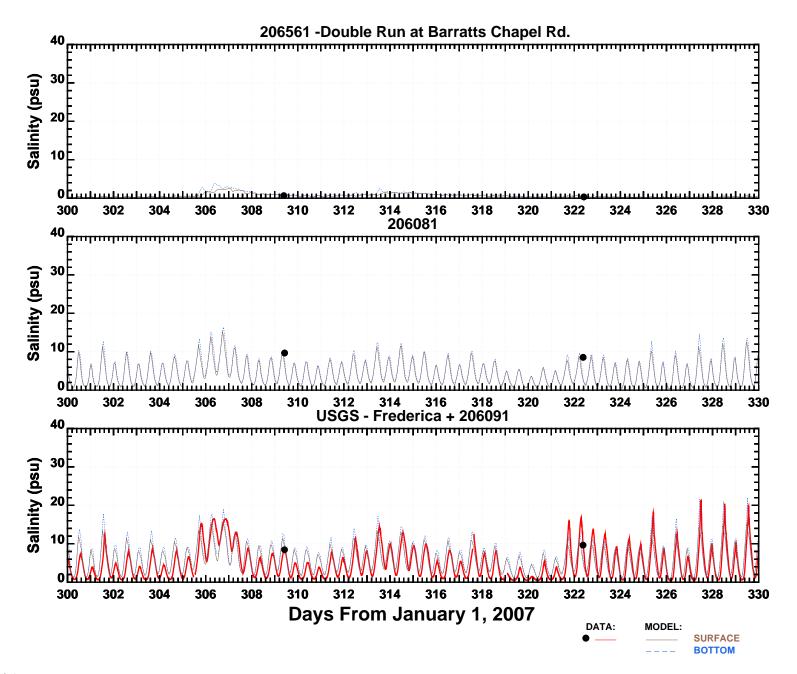


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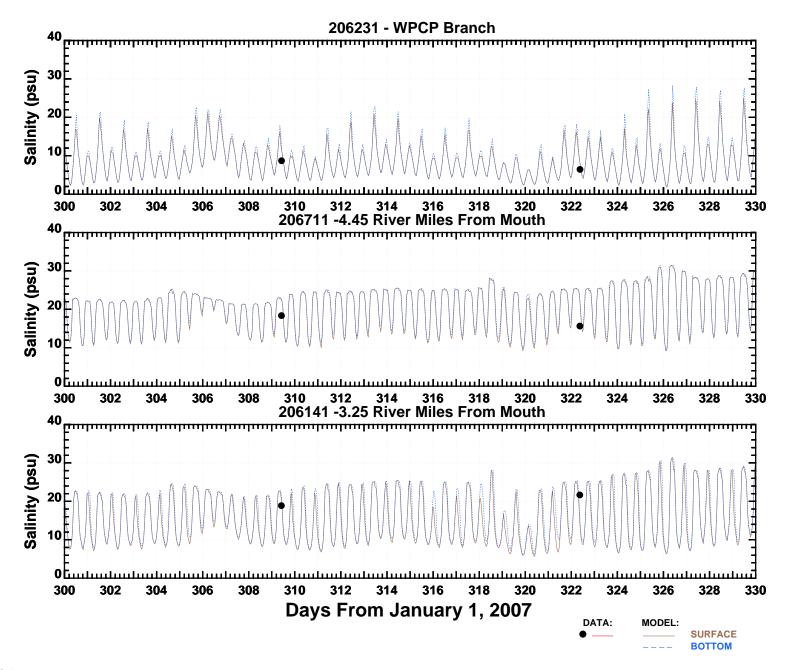
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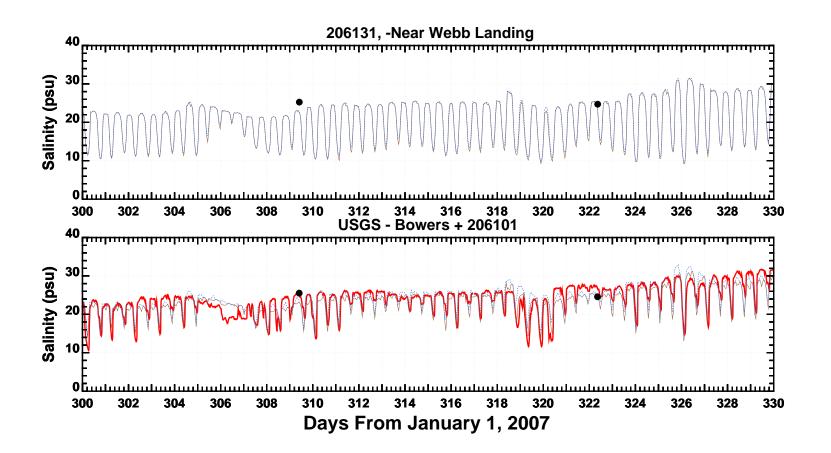
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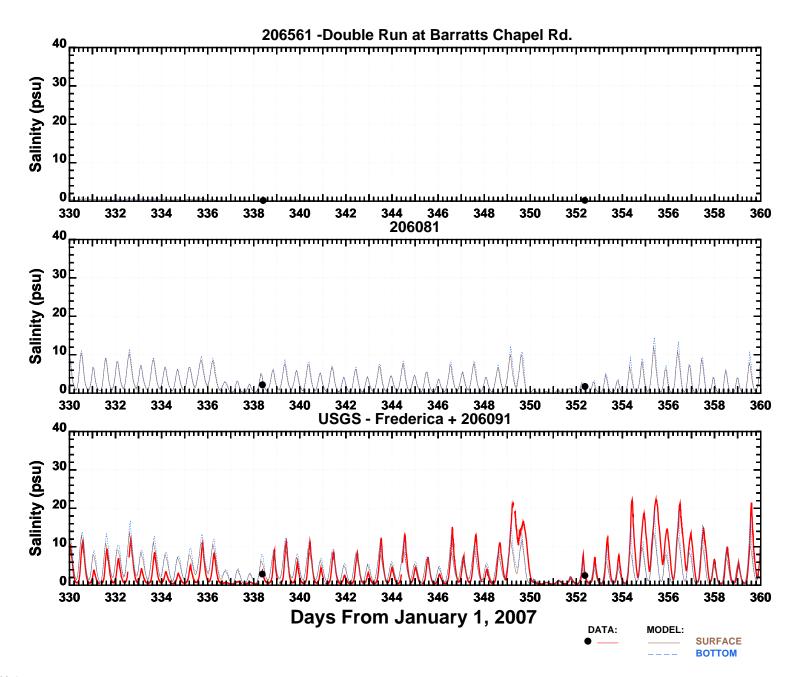


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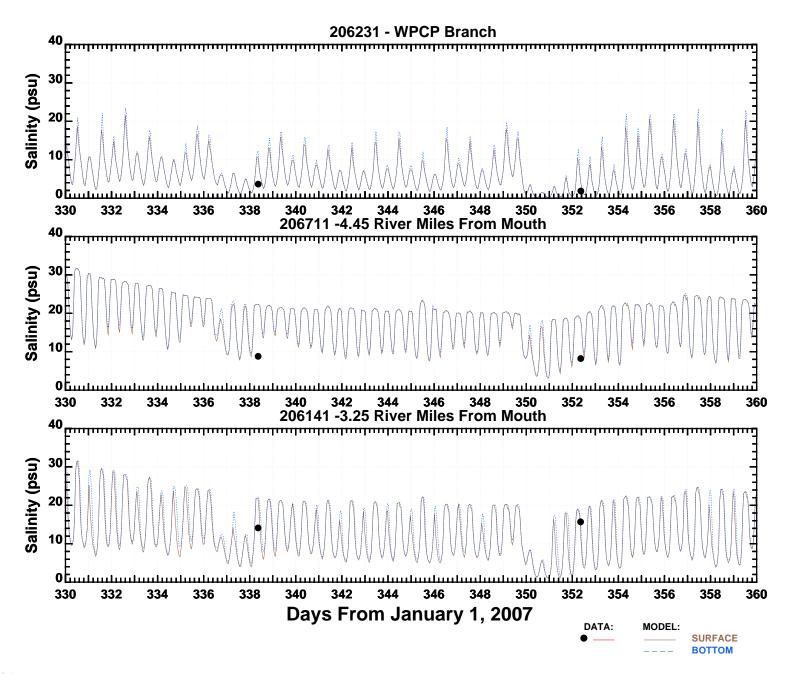
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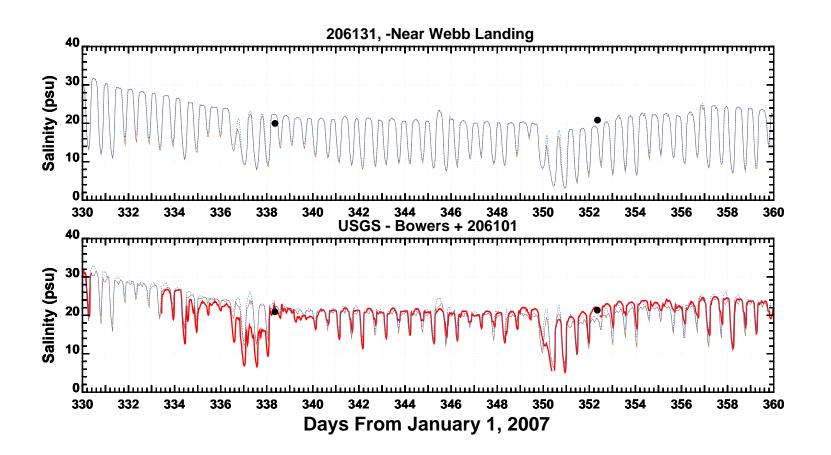
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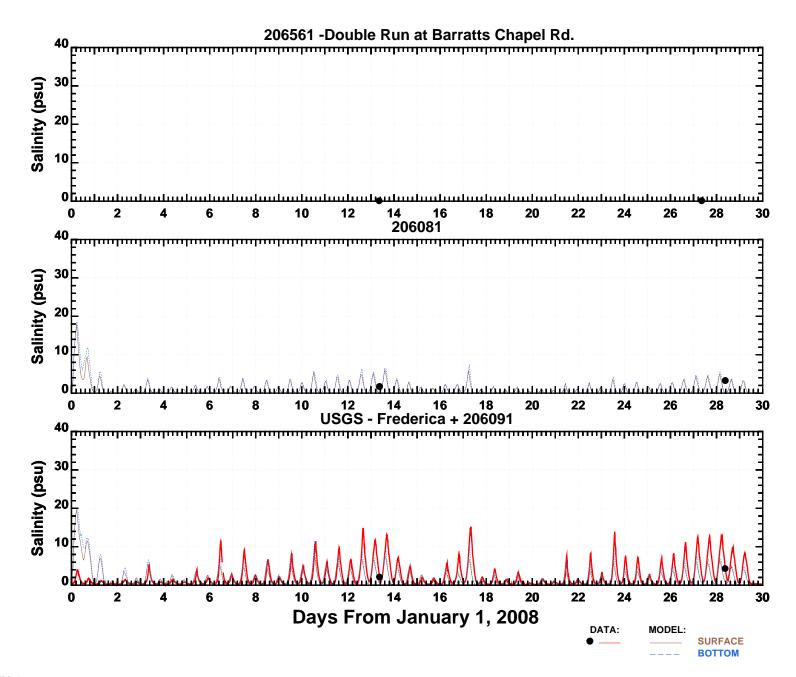
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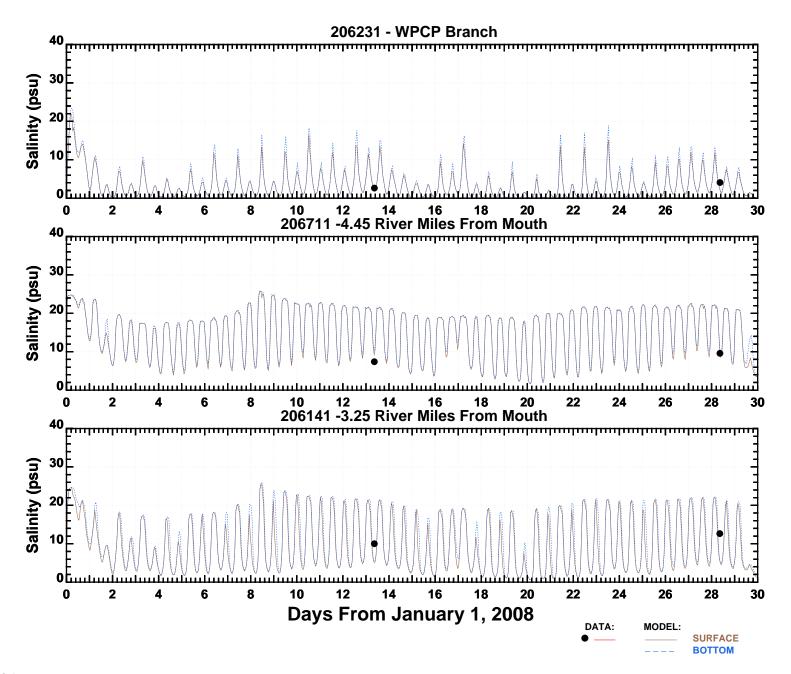


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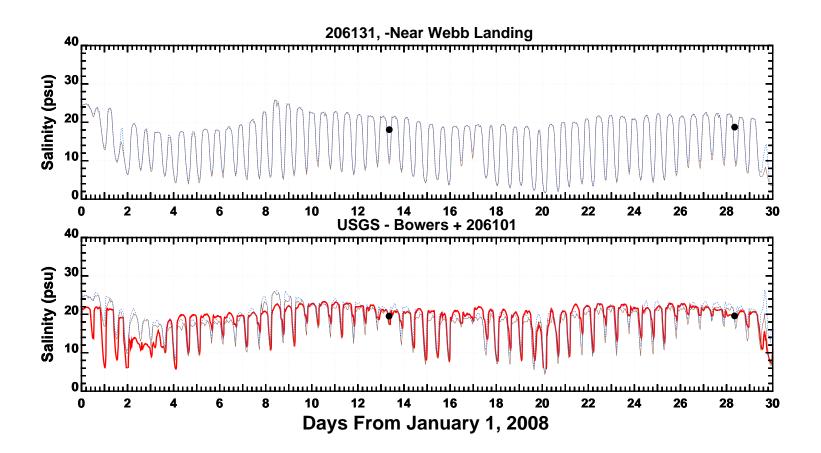


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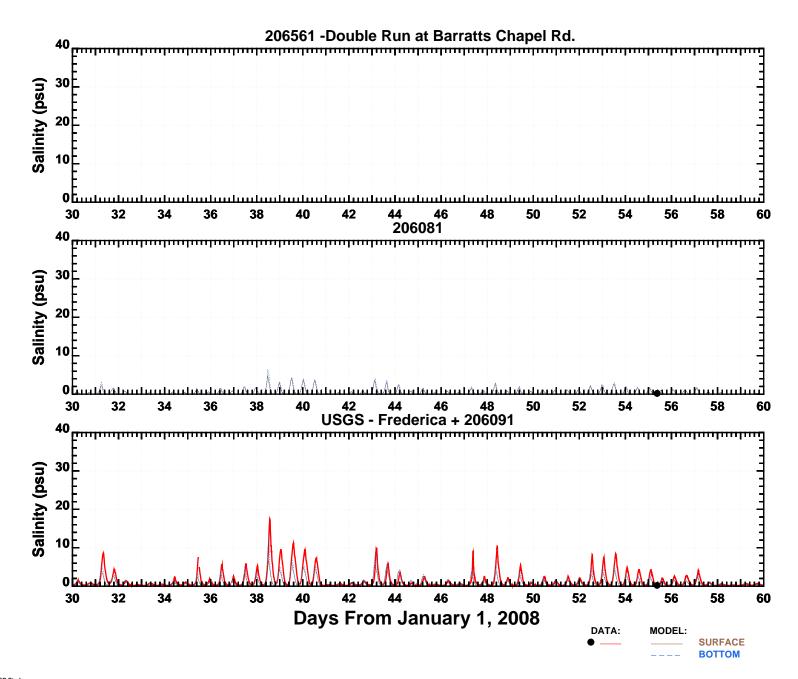
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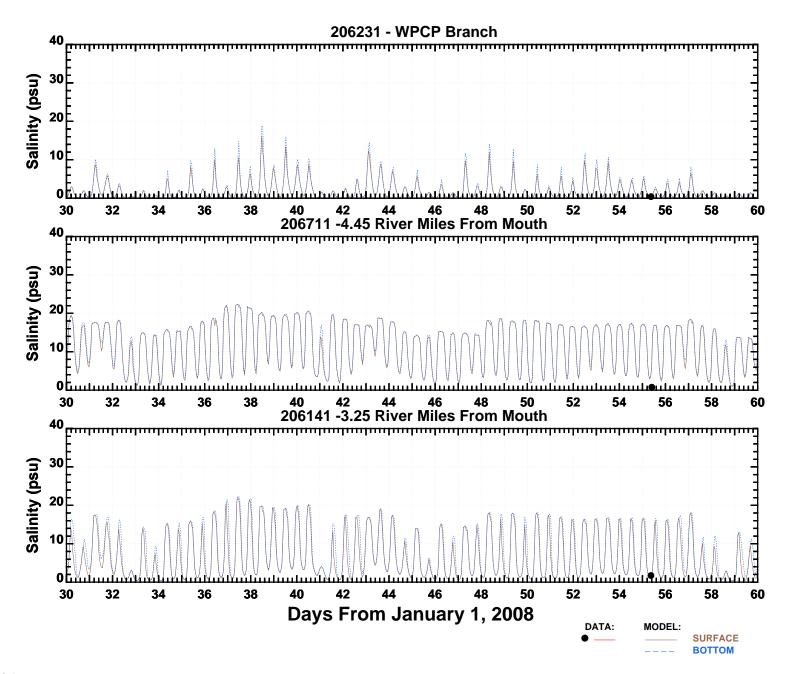


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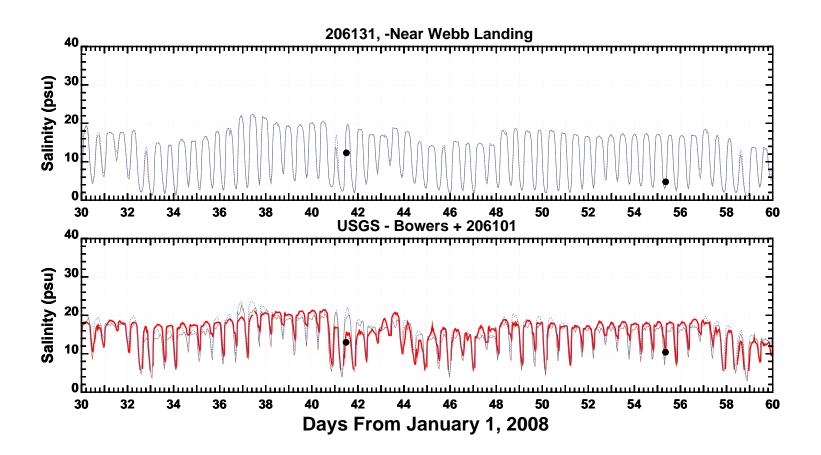


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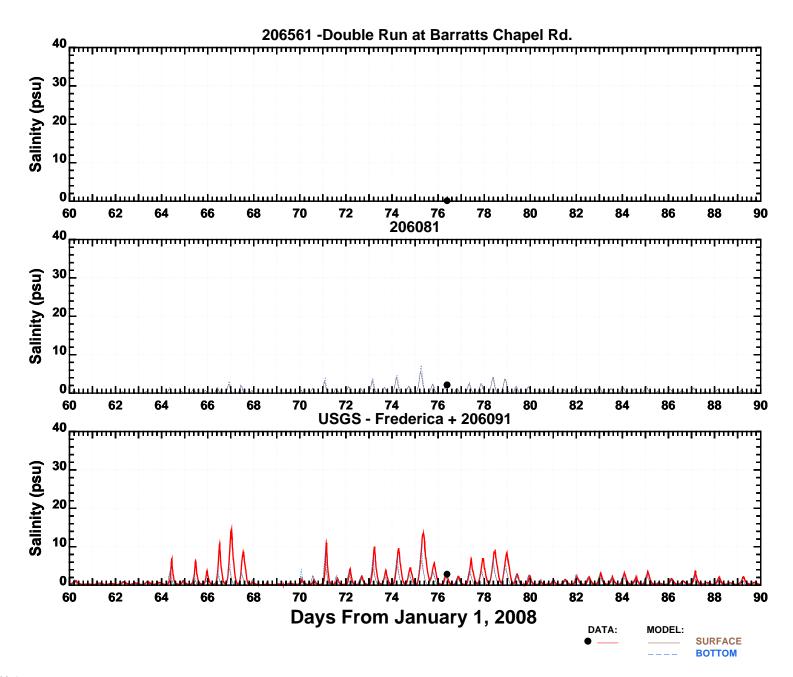
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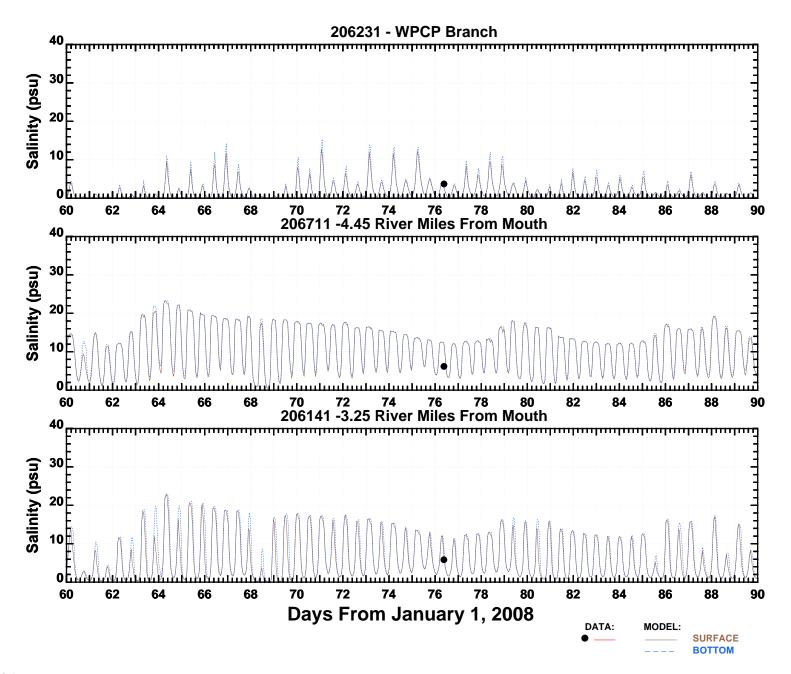


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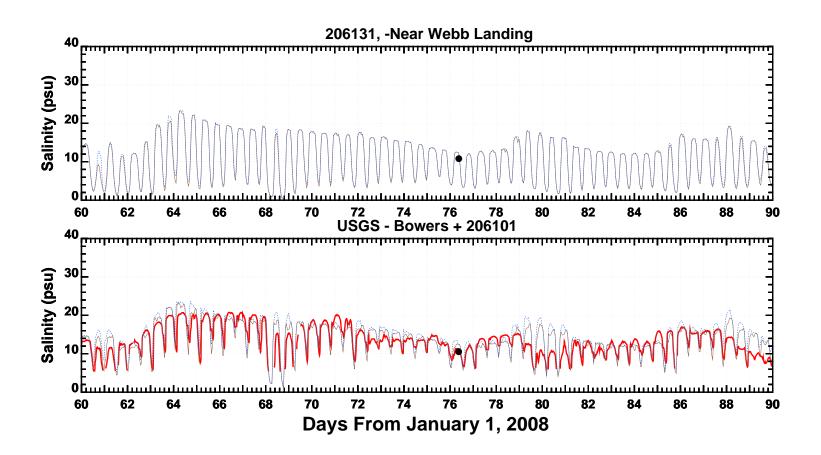


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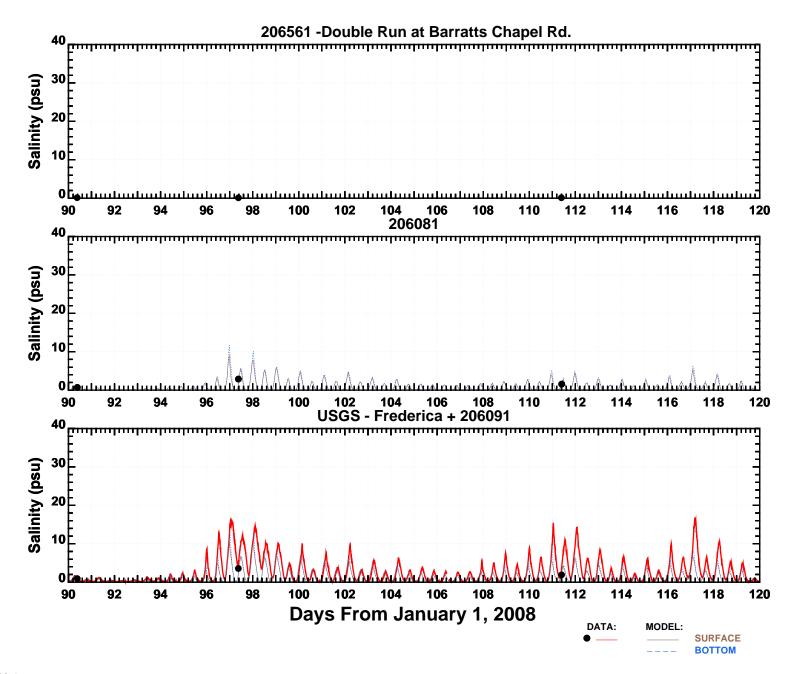
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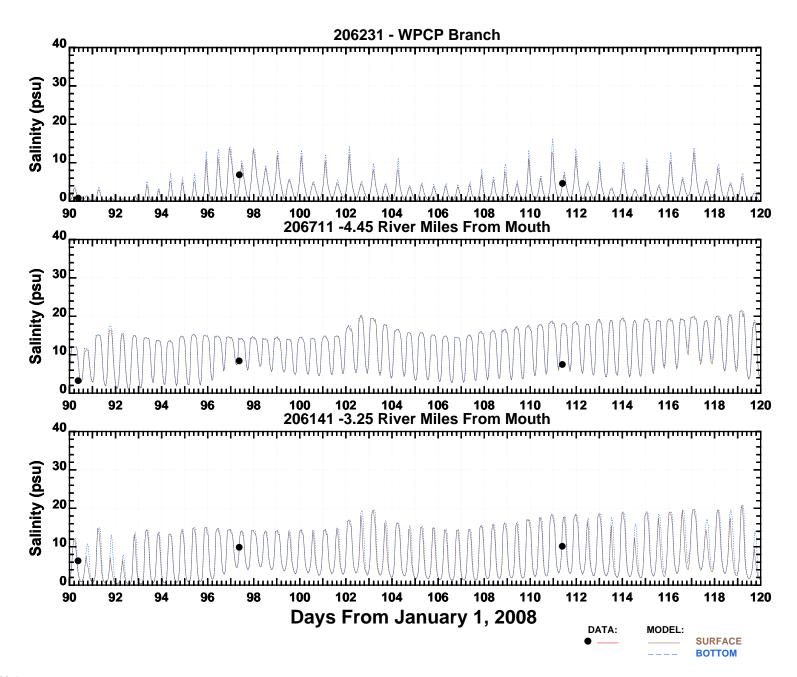


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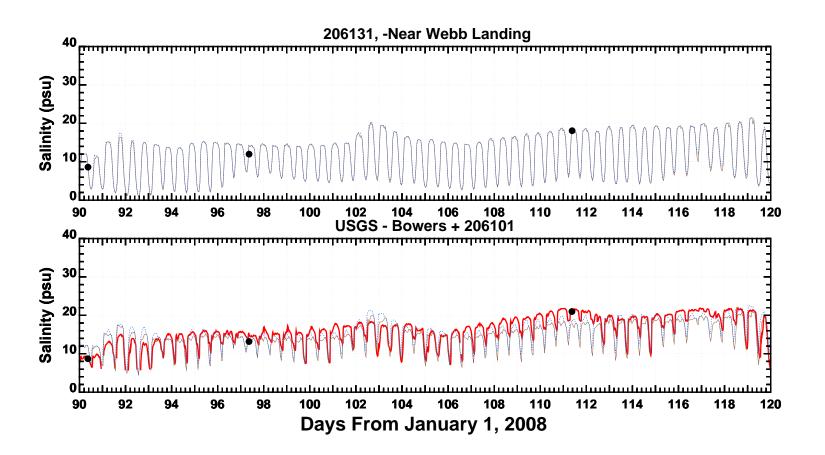


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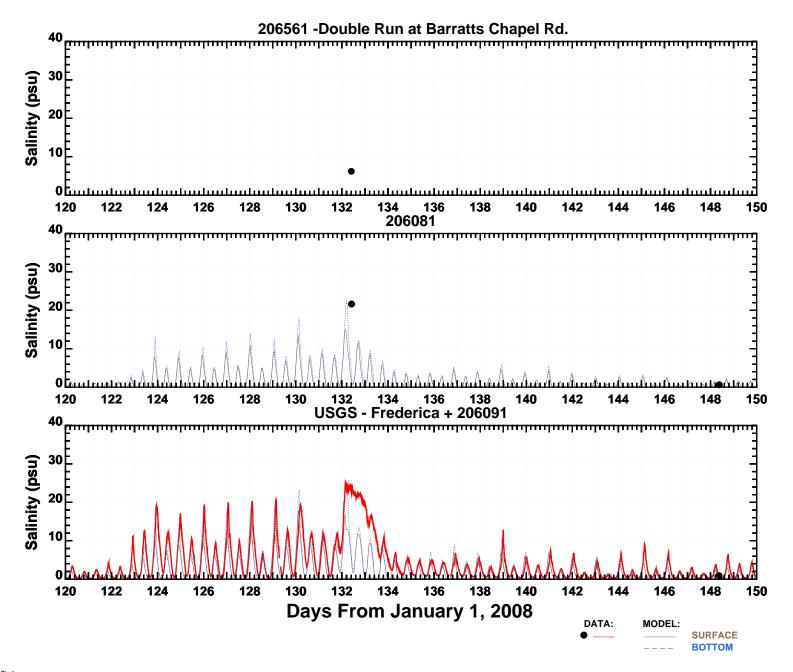


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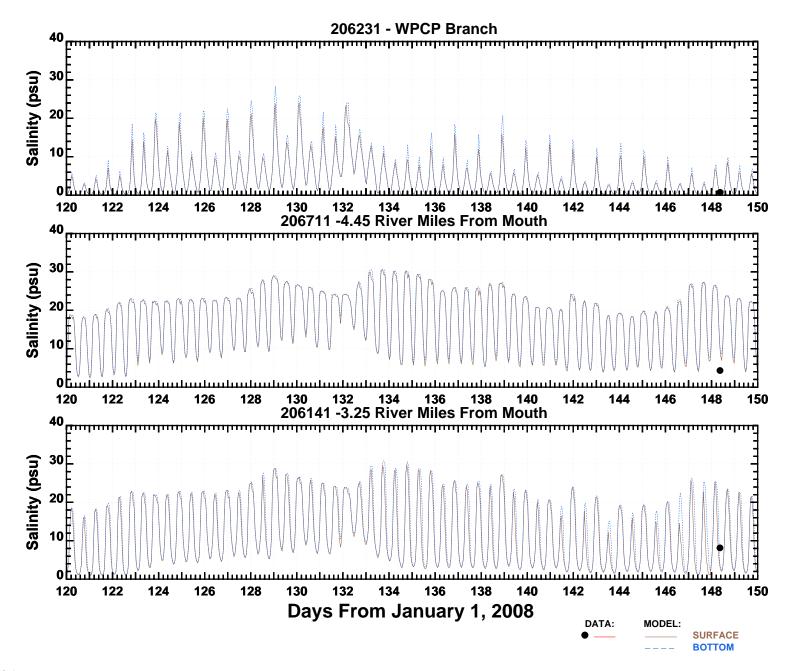


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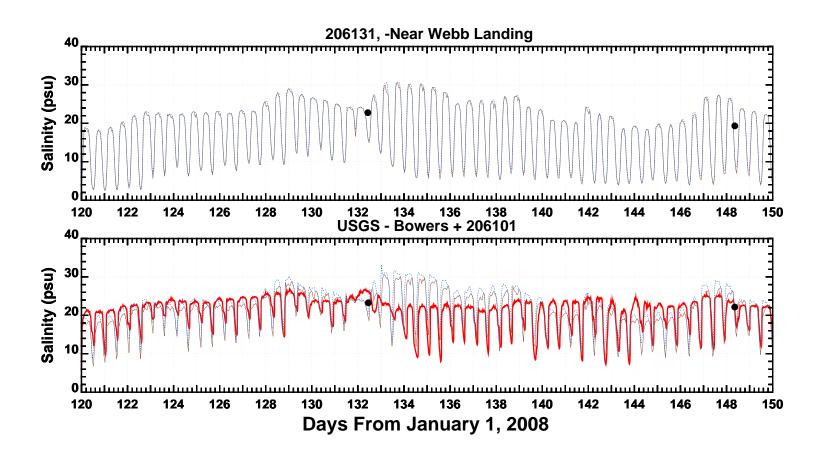
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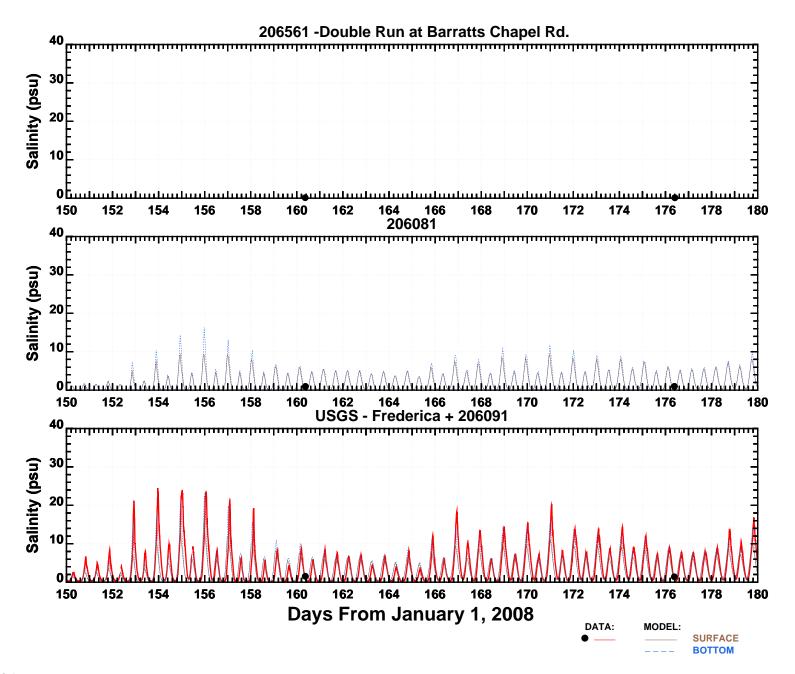


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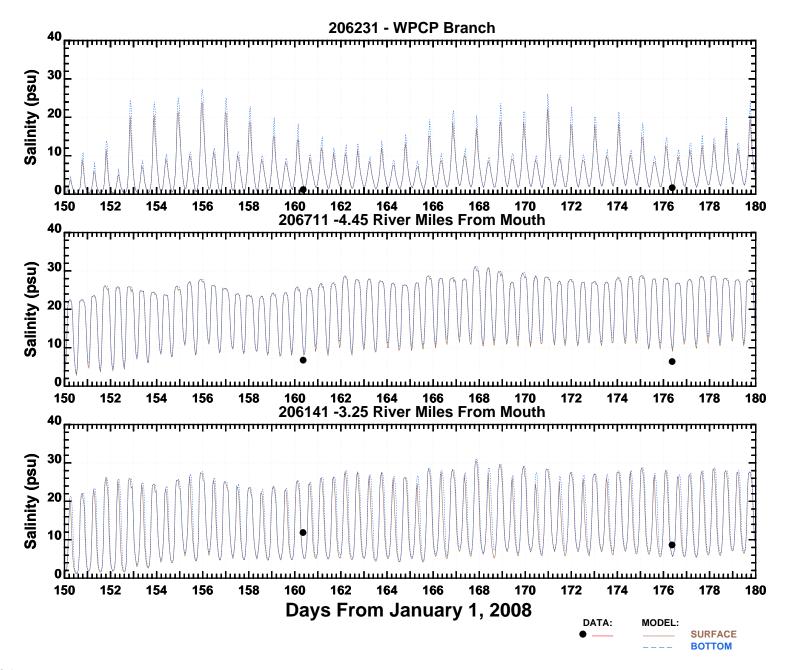
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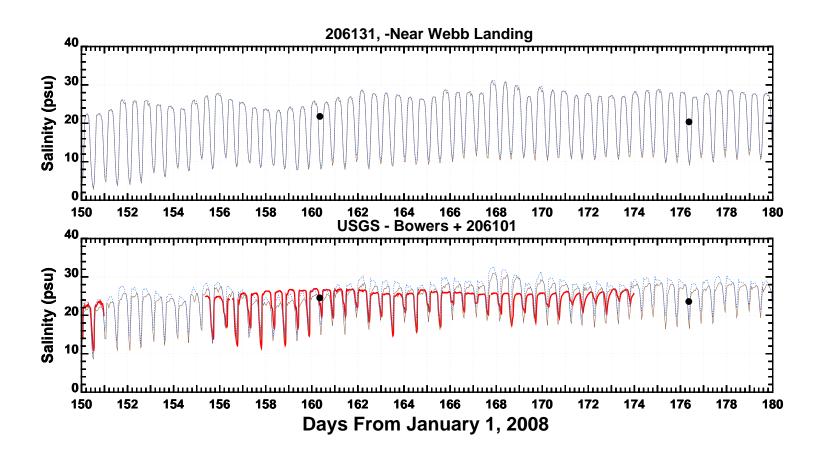
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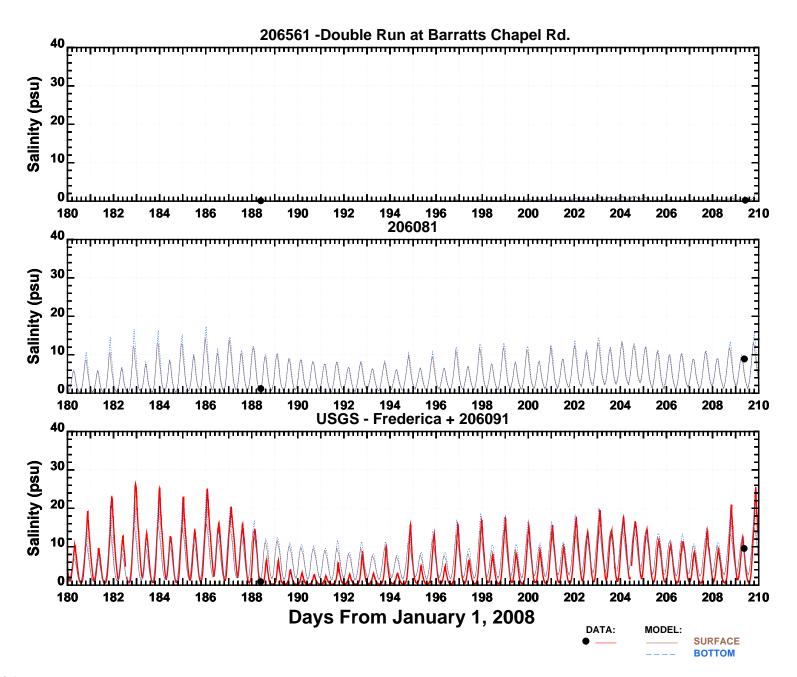


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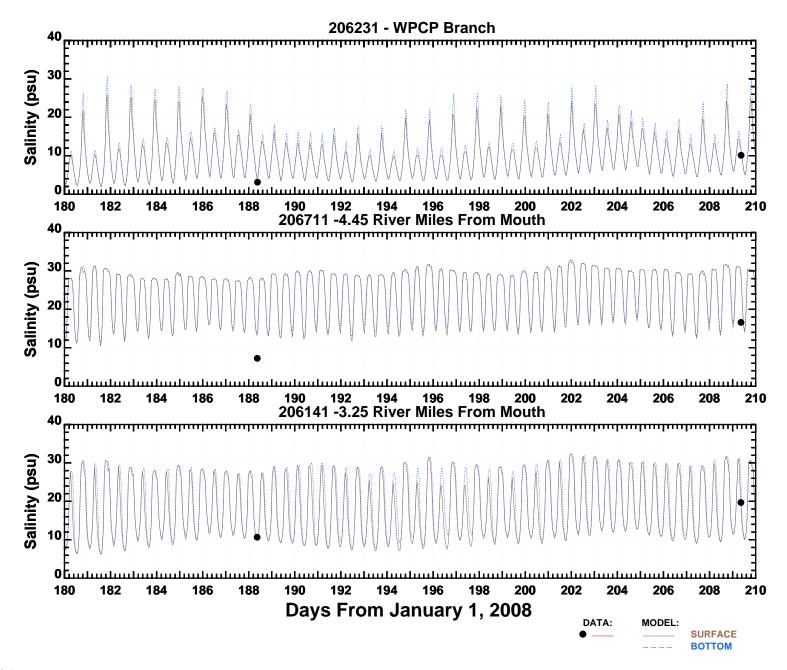
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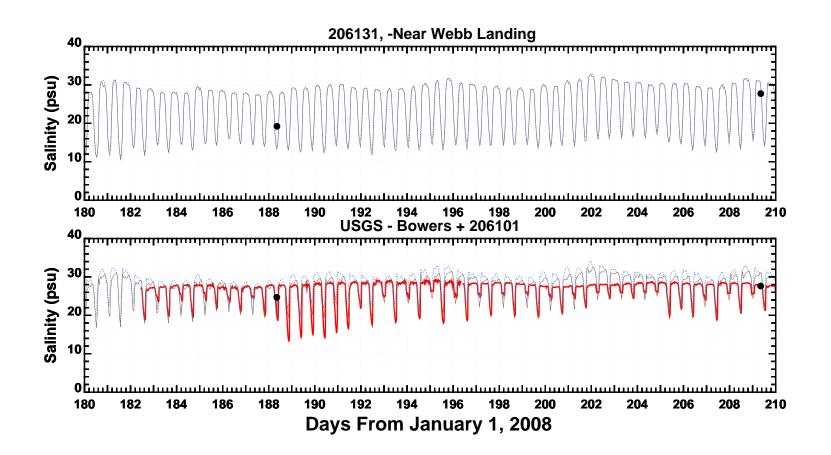
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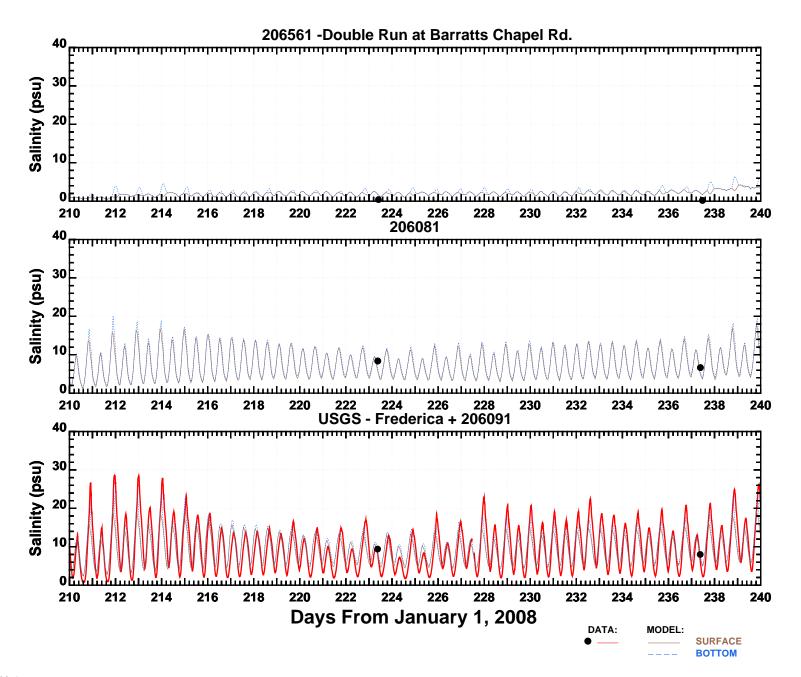


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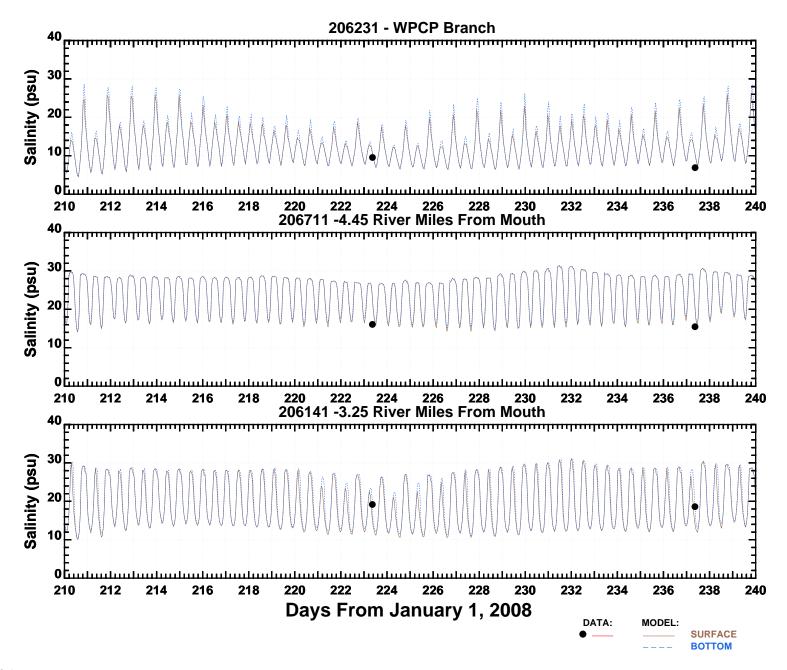
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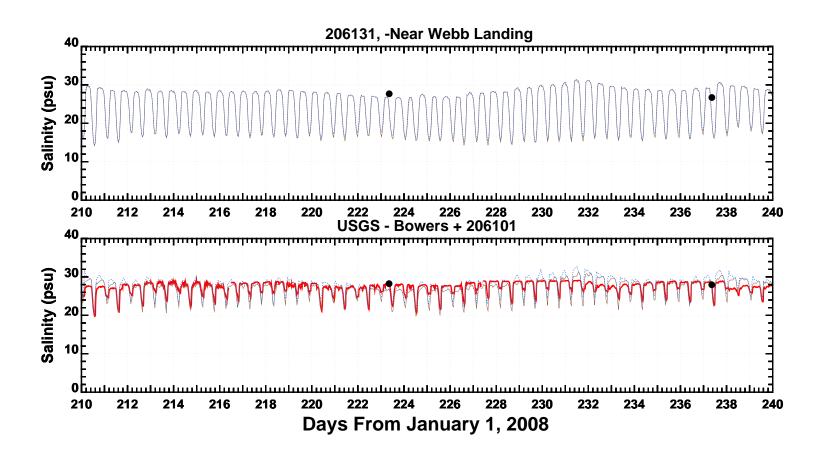
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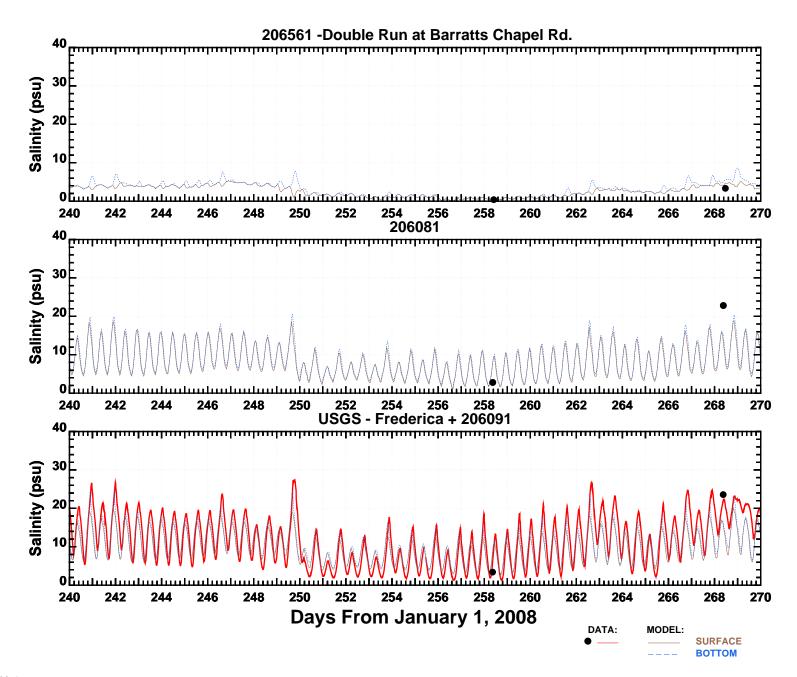


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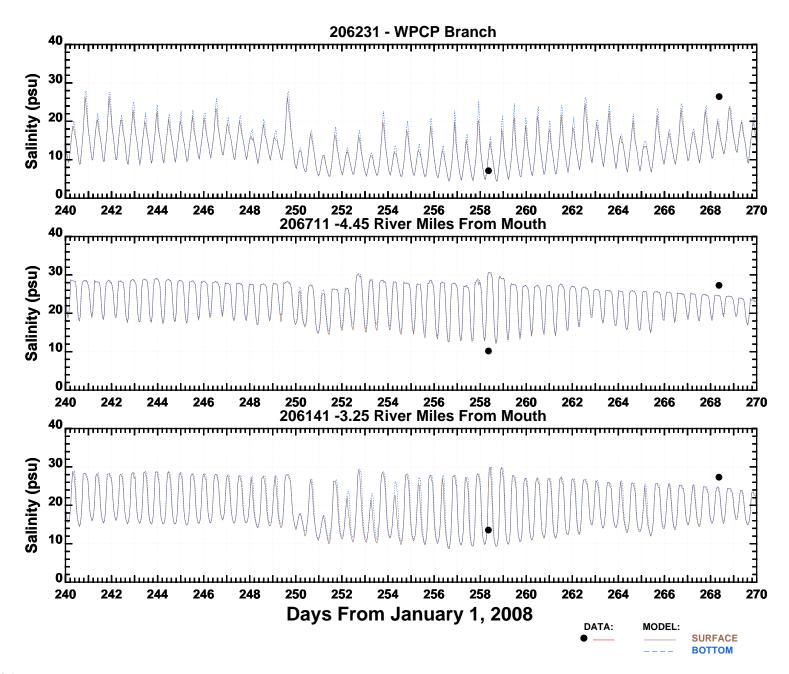
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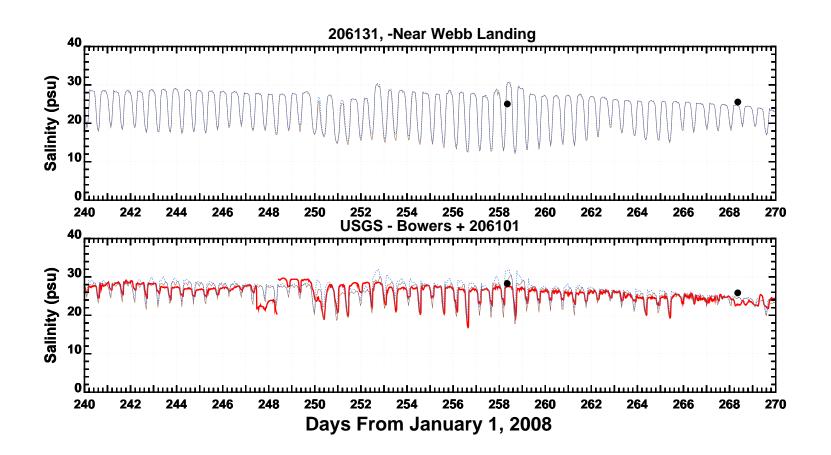
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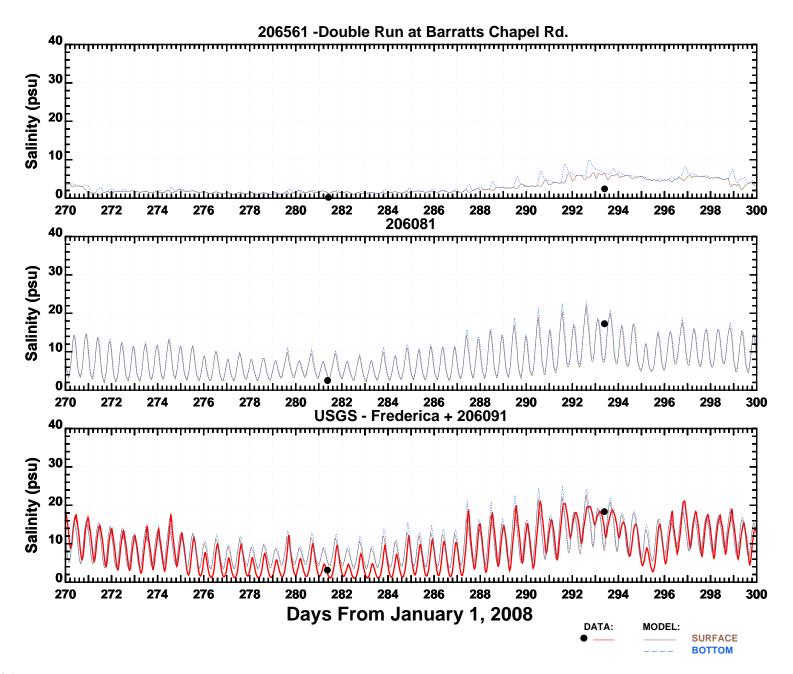
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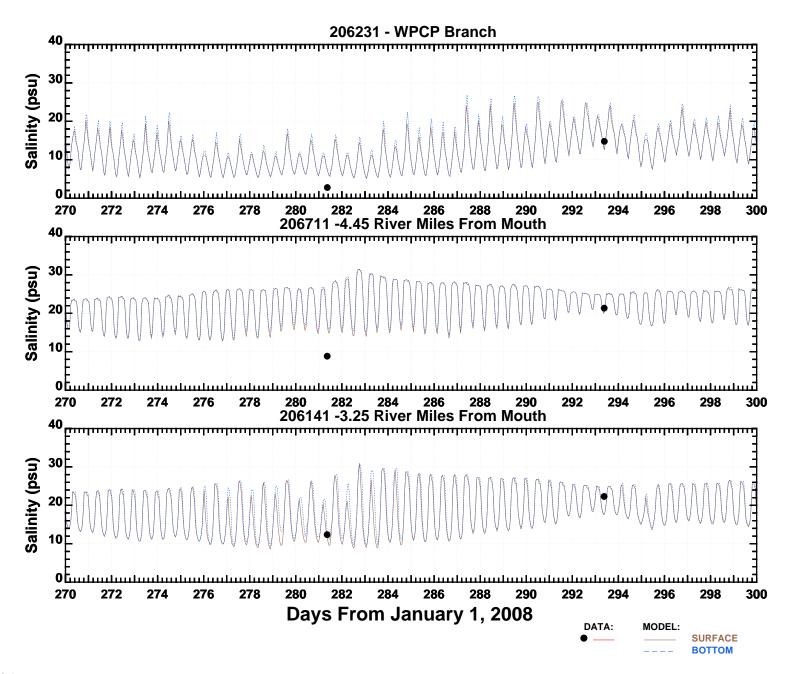
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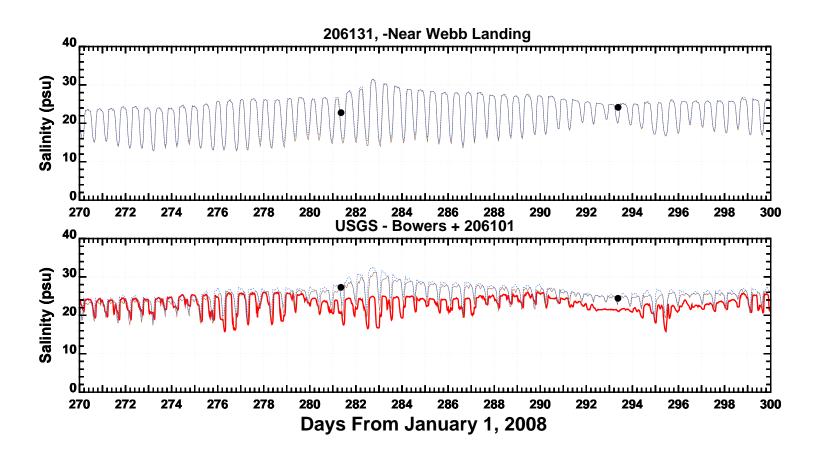
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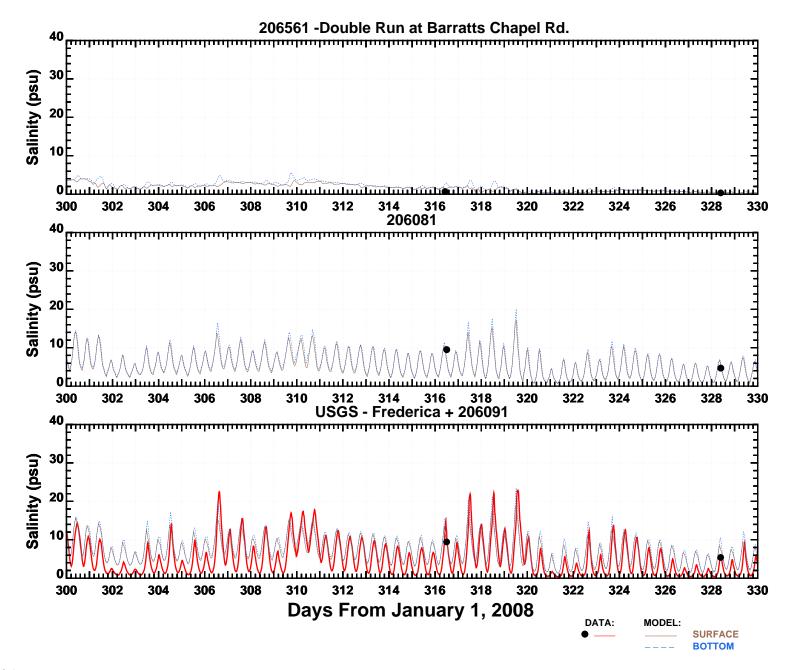


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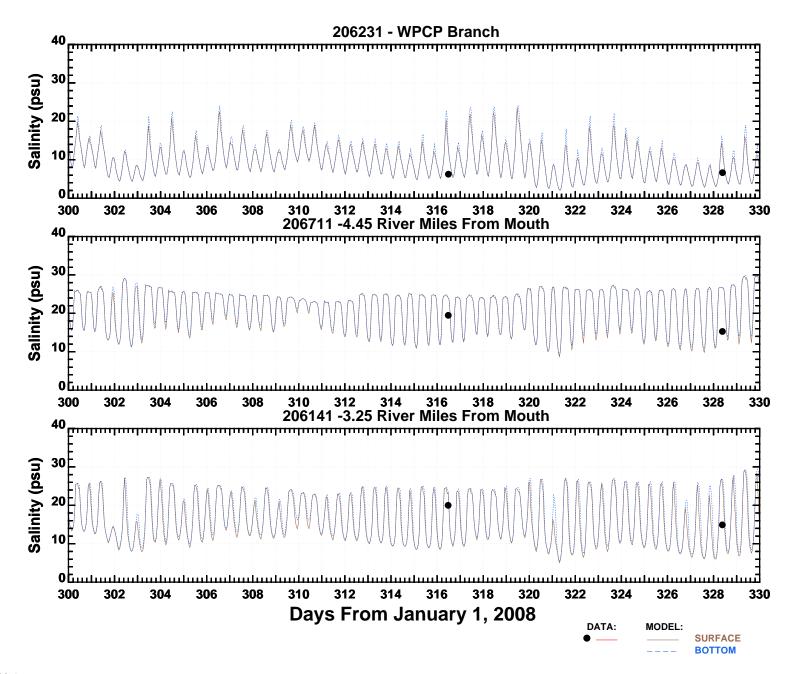
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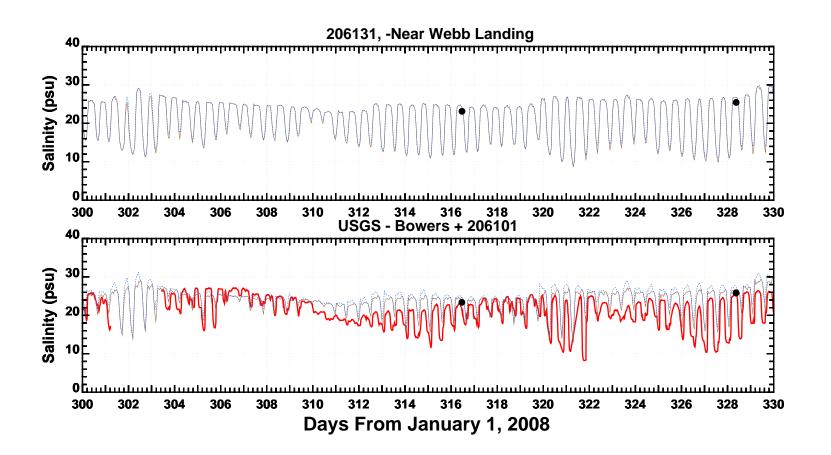
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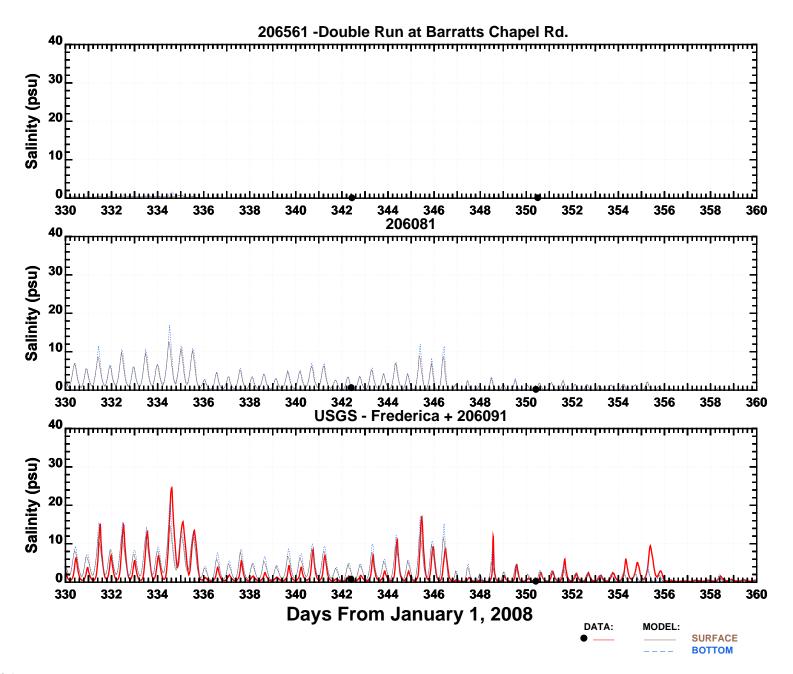


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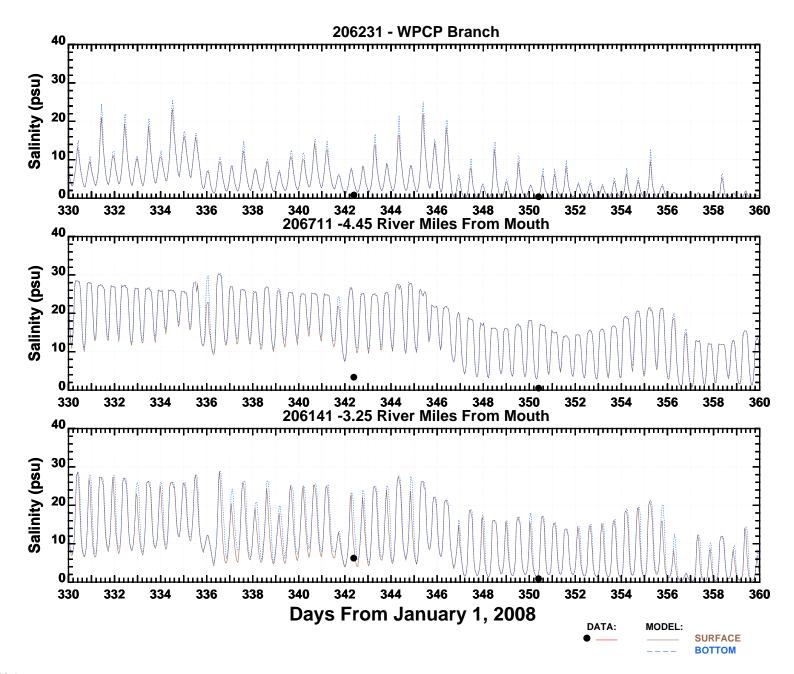
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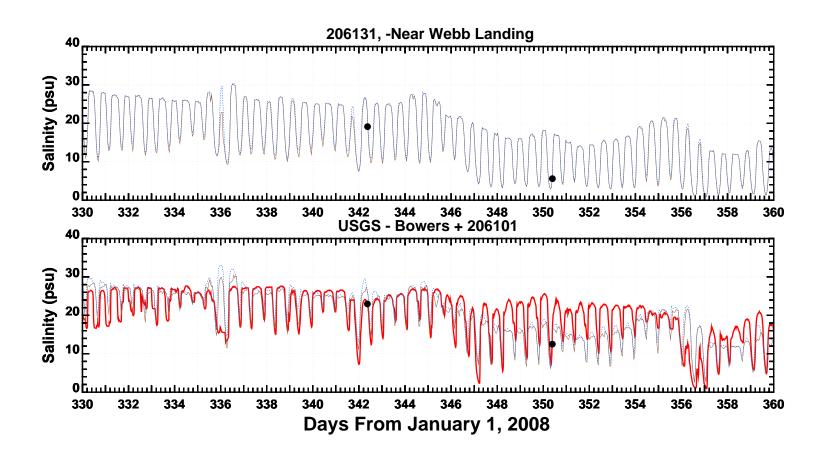
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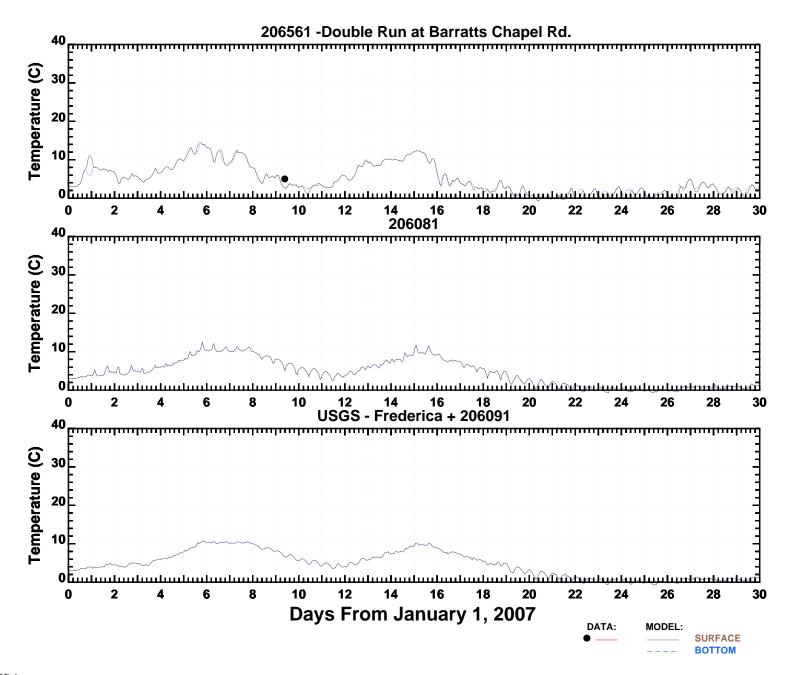


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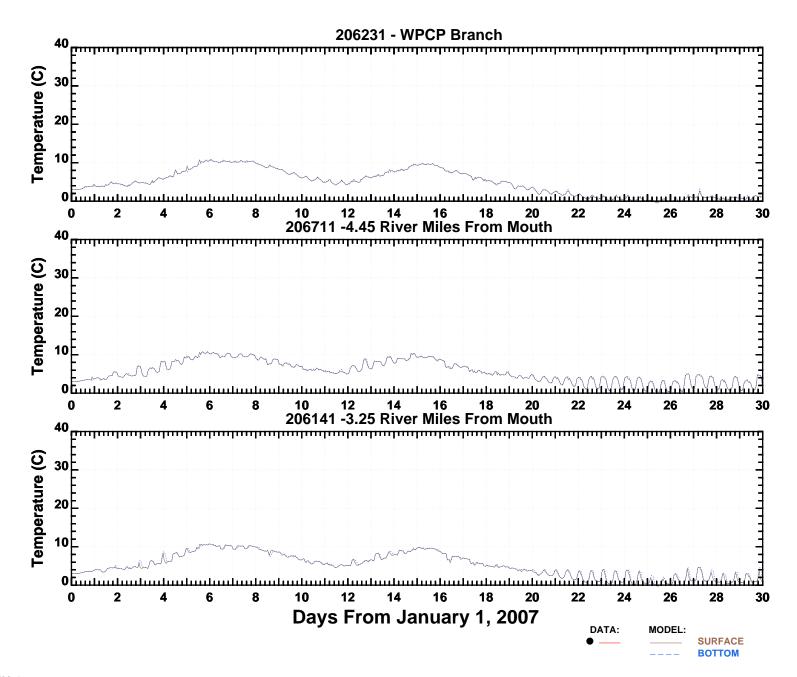


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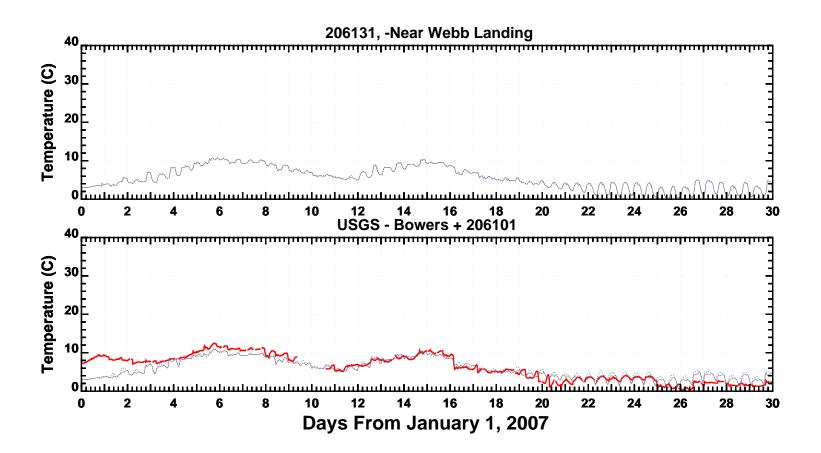


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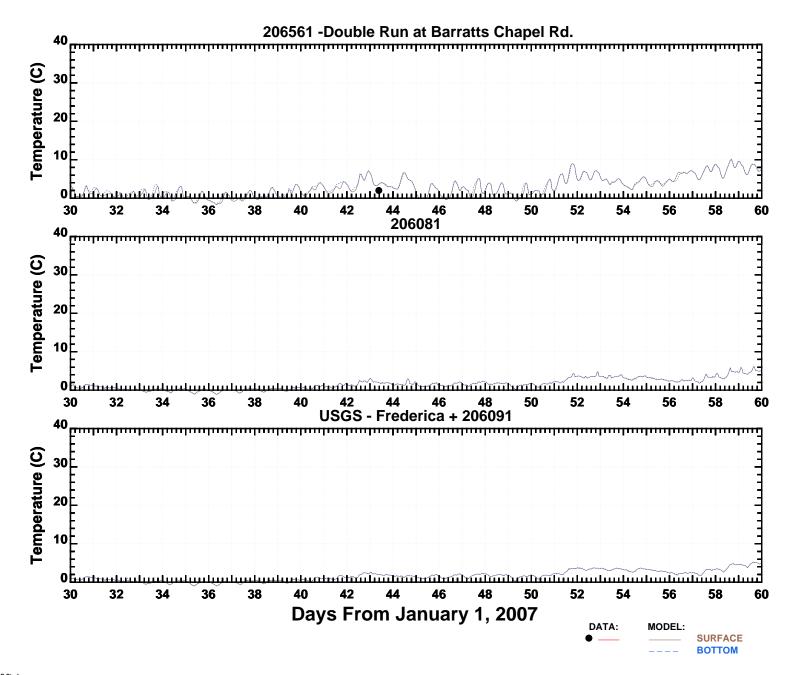


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RUN031: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flowp.

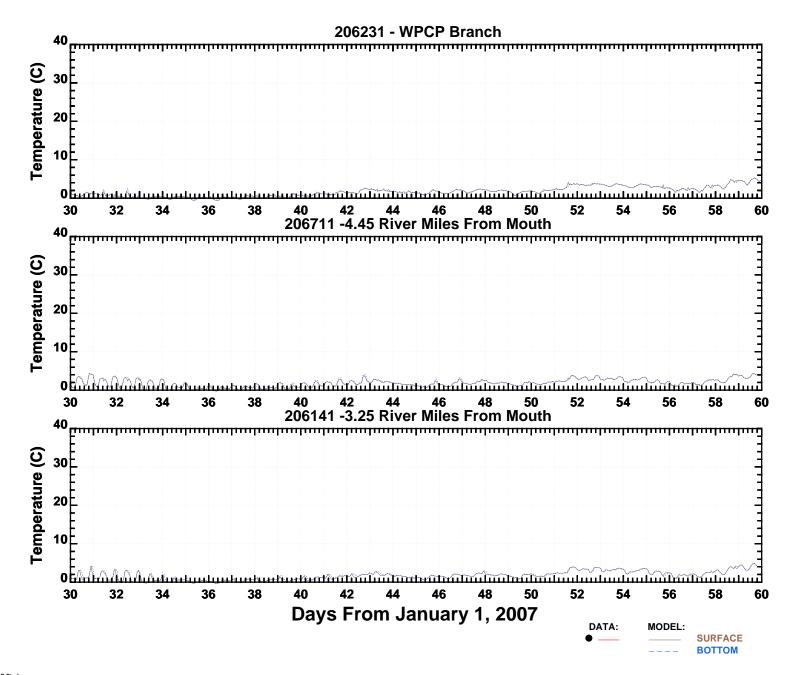


DNREC Study

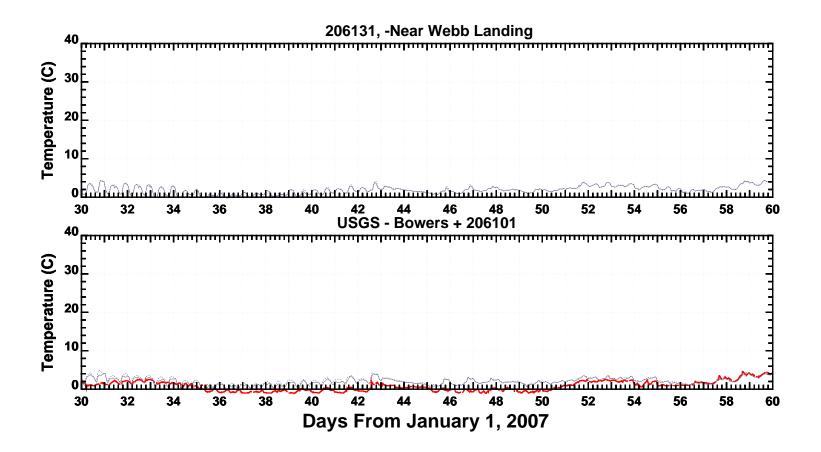
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RUN031: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flowp

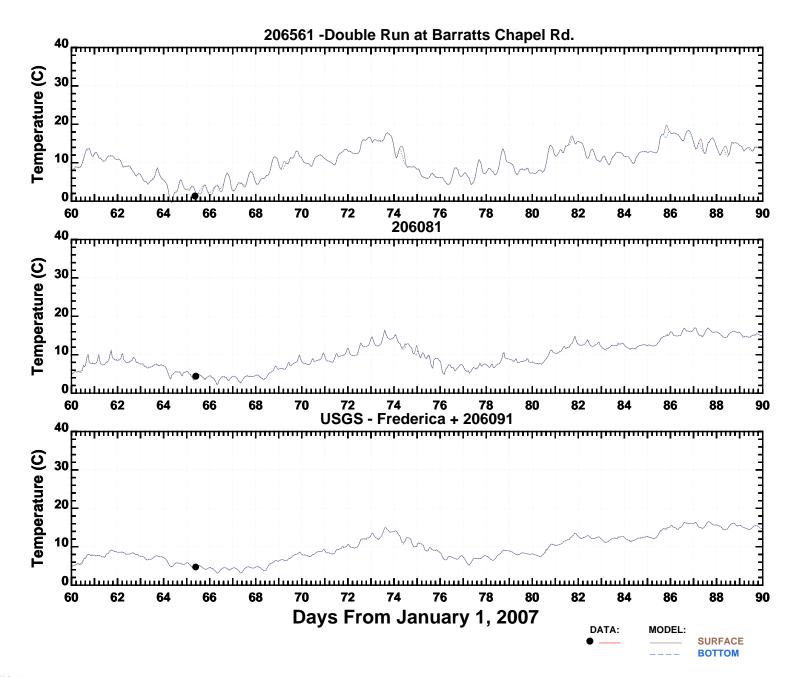


DNREC Study
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RUN031: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flowp.



DATA: MODEL:

SURFACE
BOTTOM

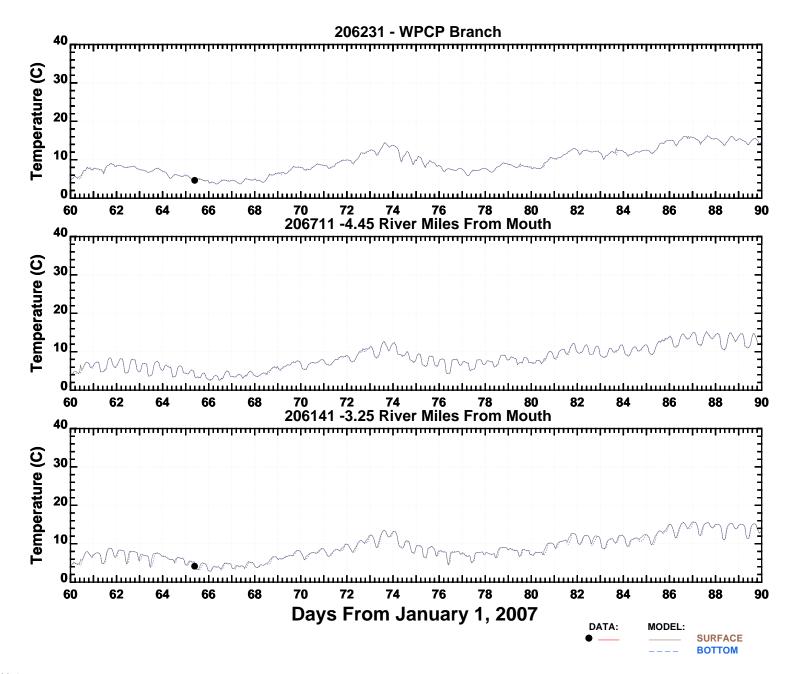


DNREC Study

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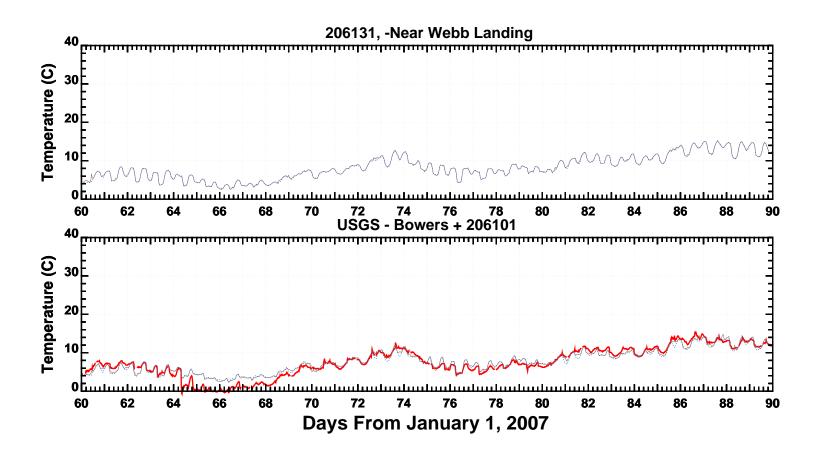


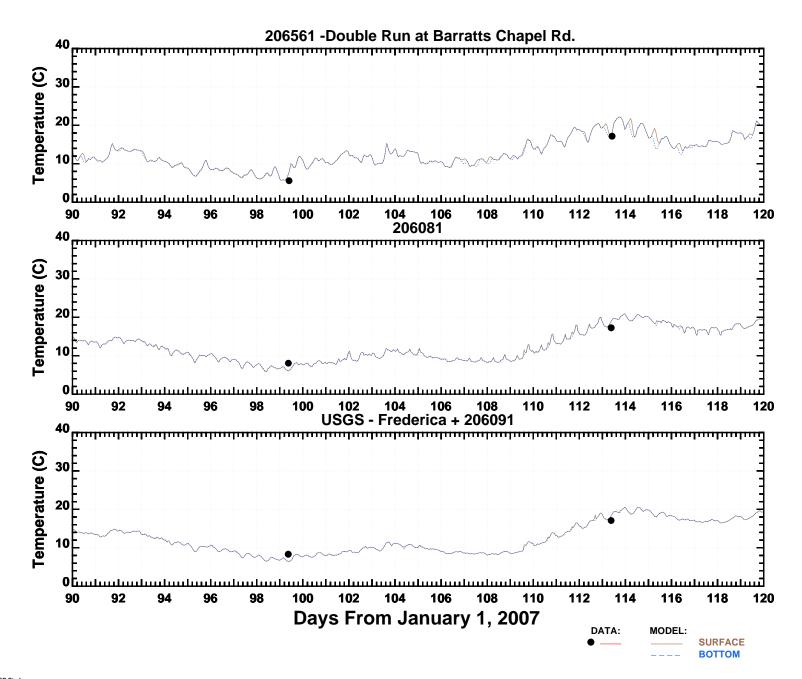
DNREC Study

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RUN031: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flowp.



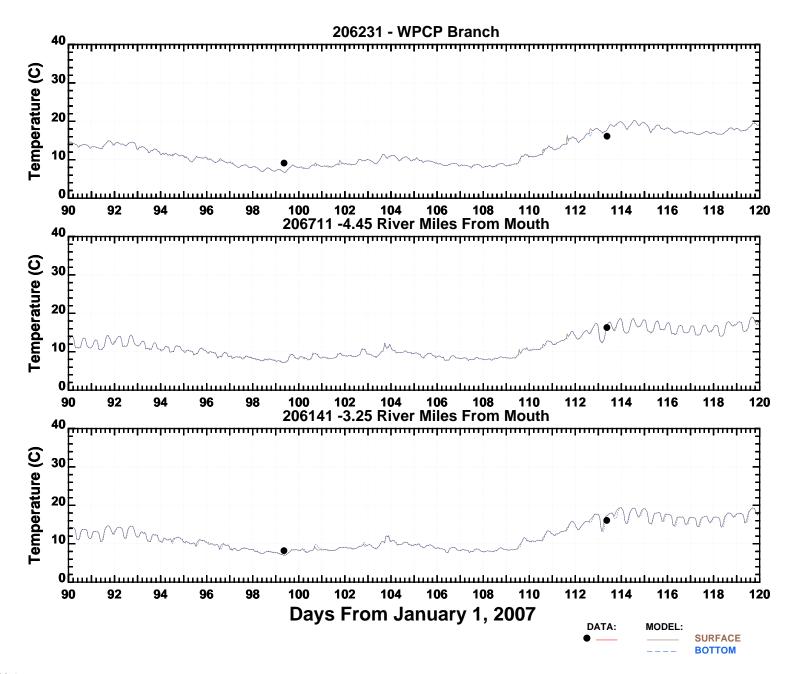


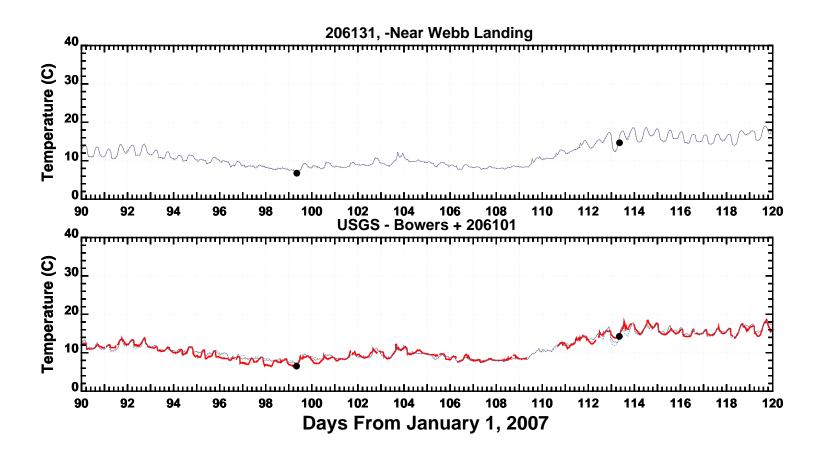
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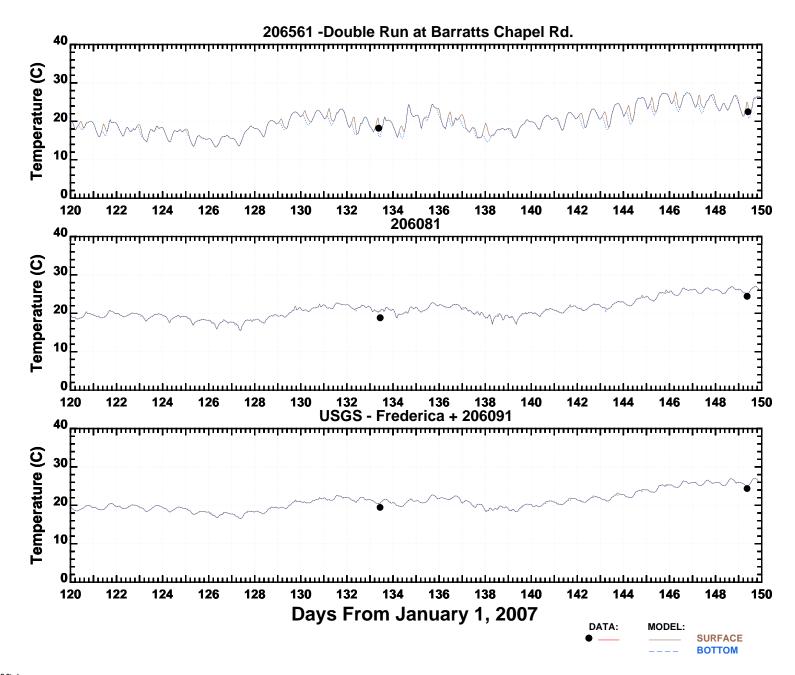
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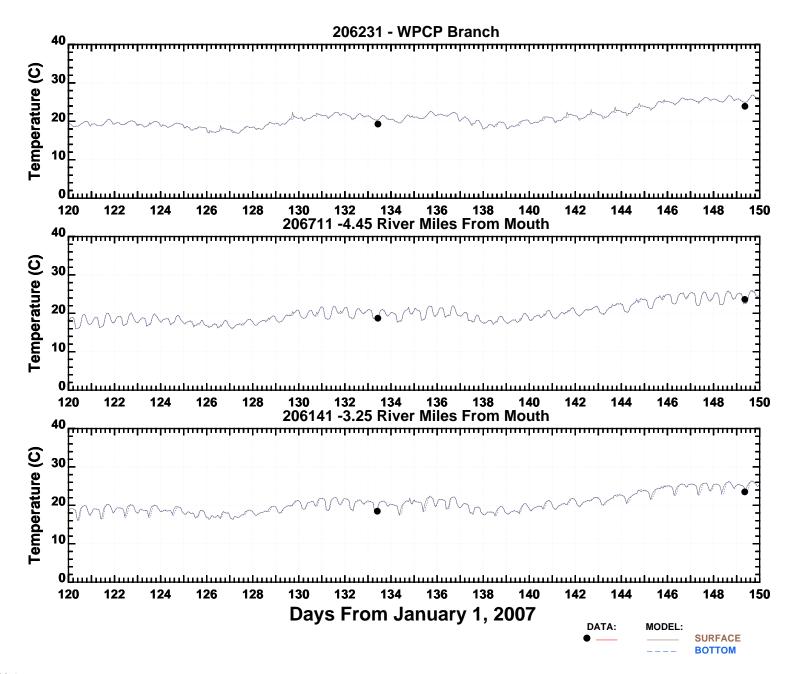
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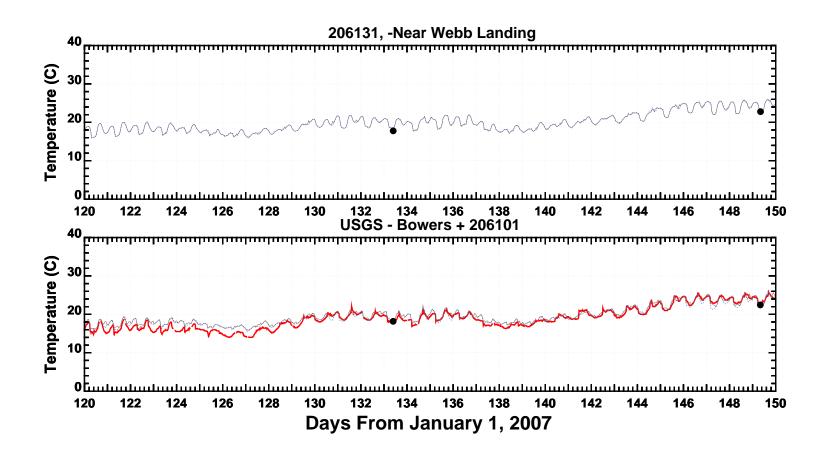
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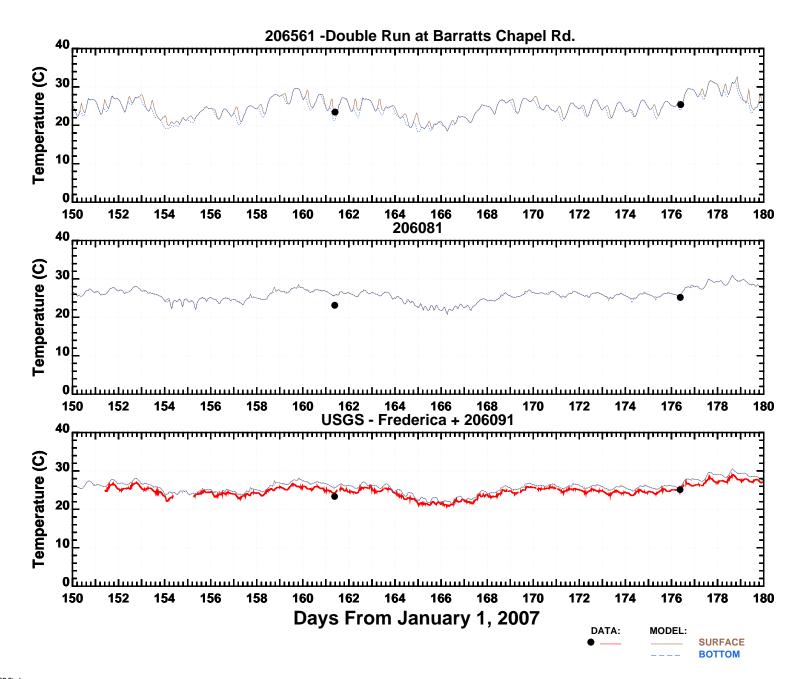


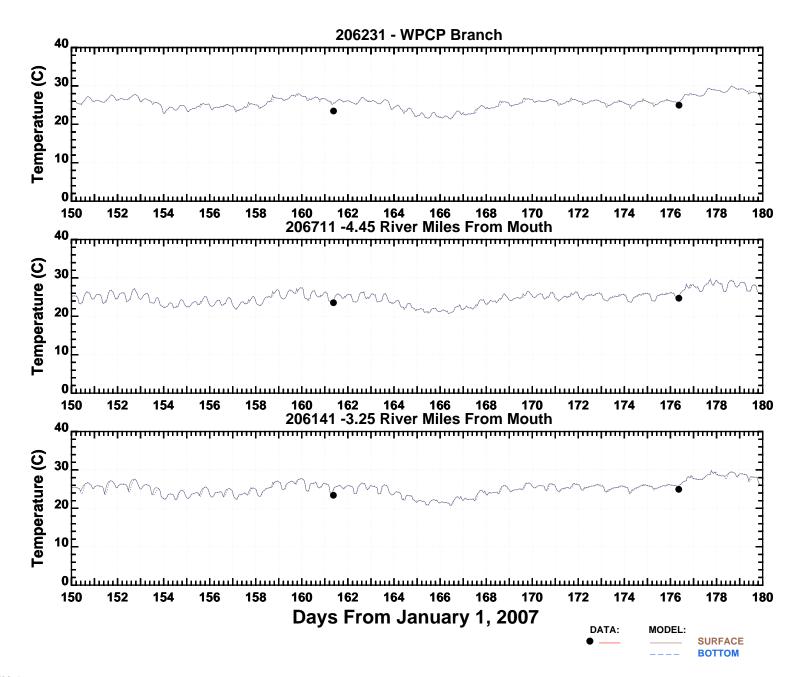


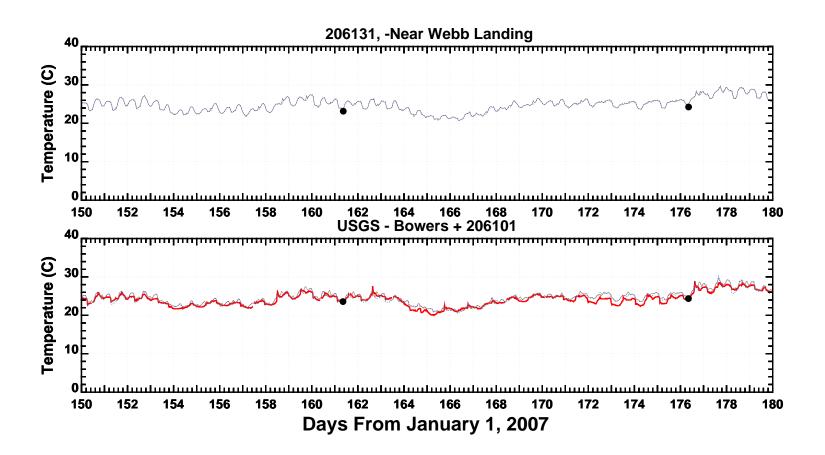


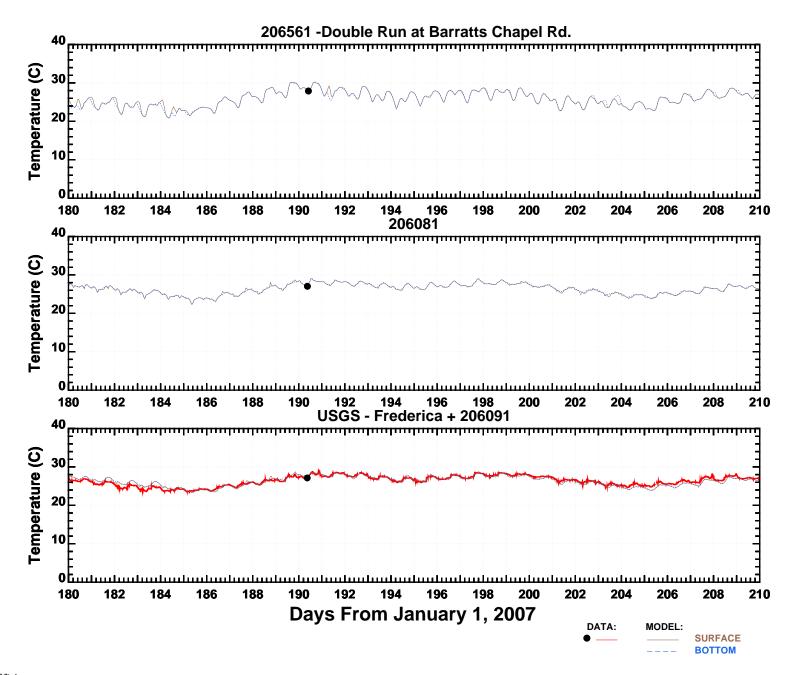


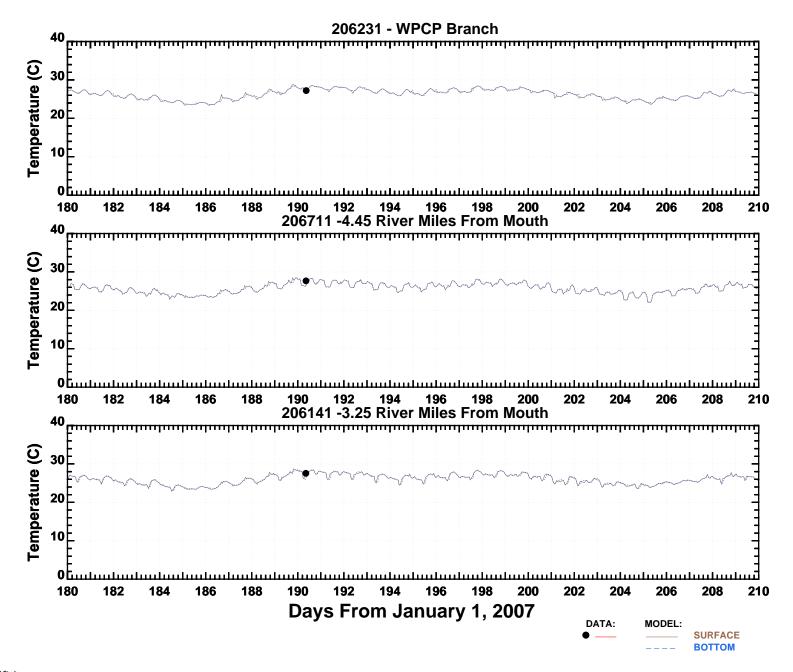


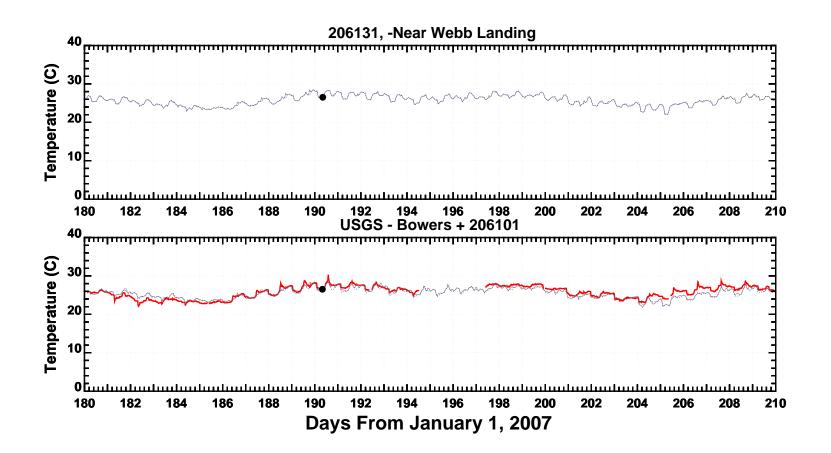


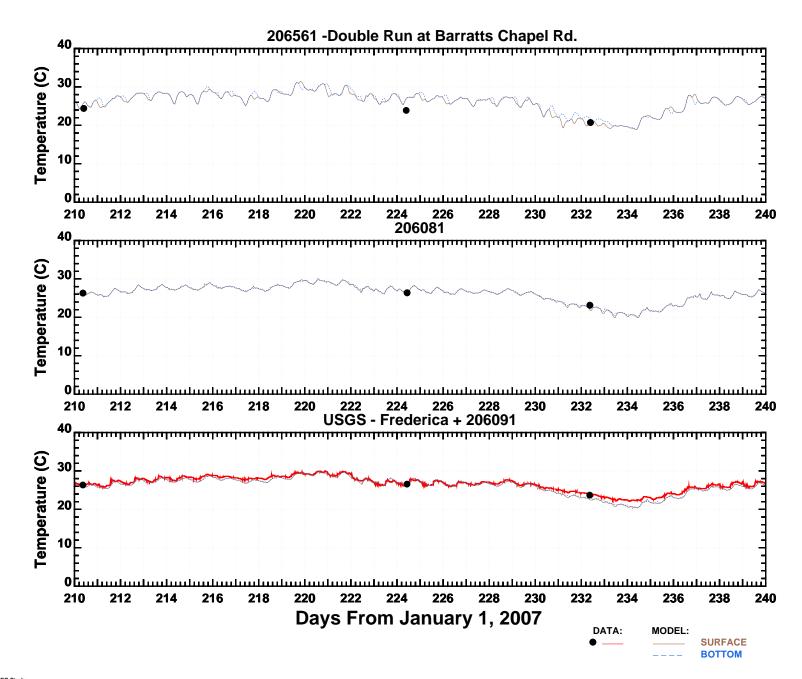


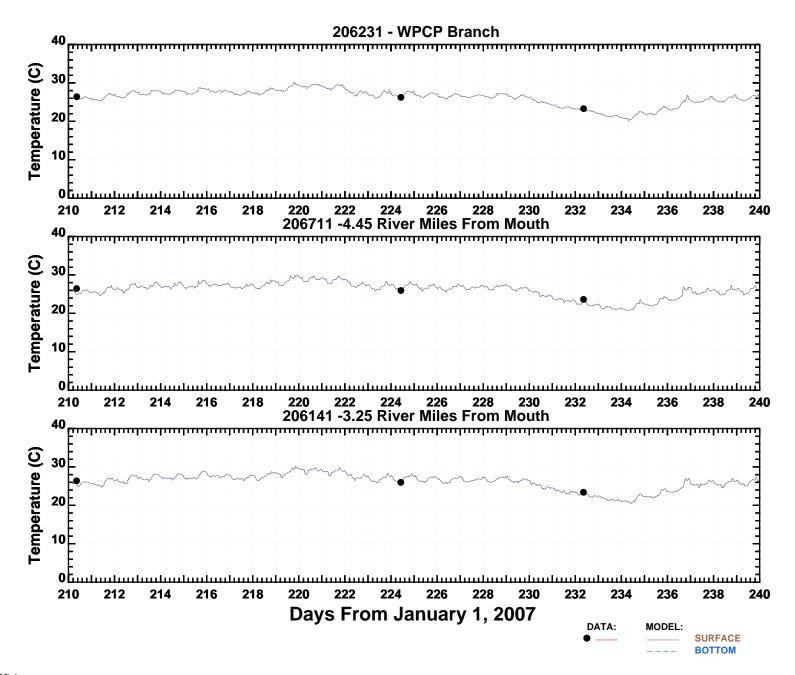


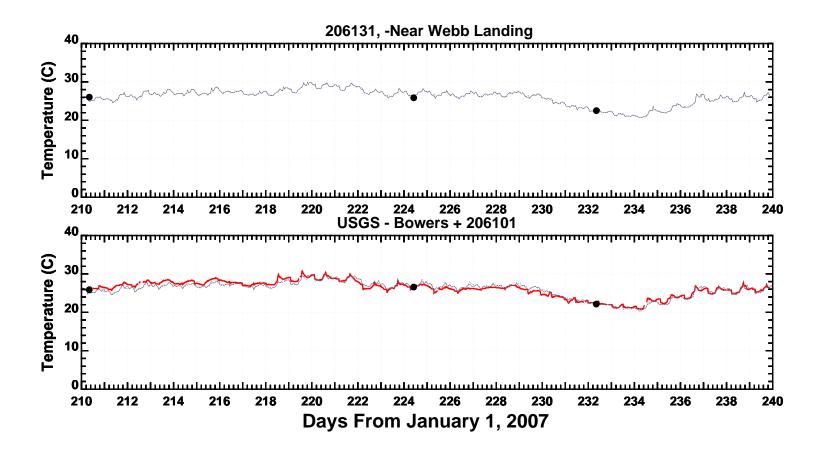


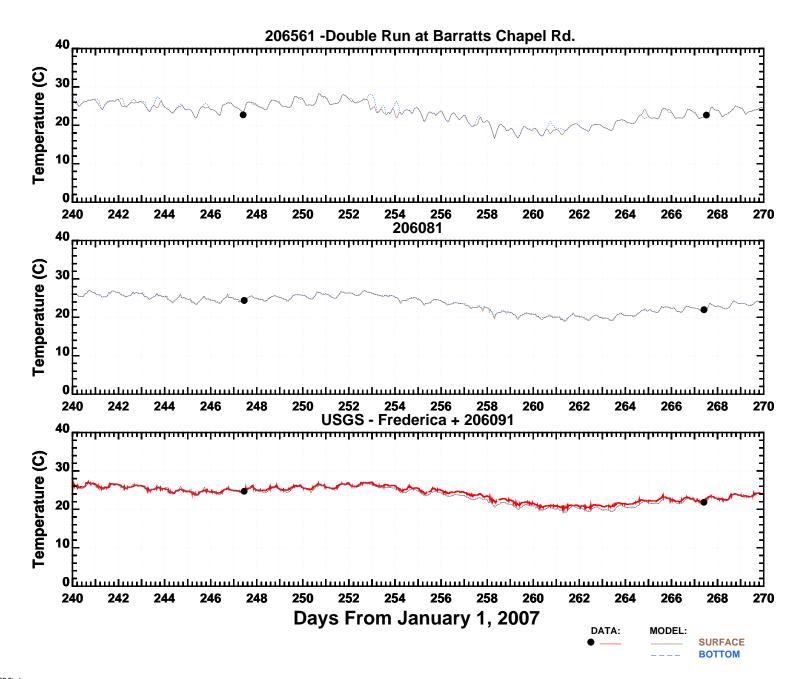


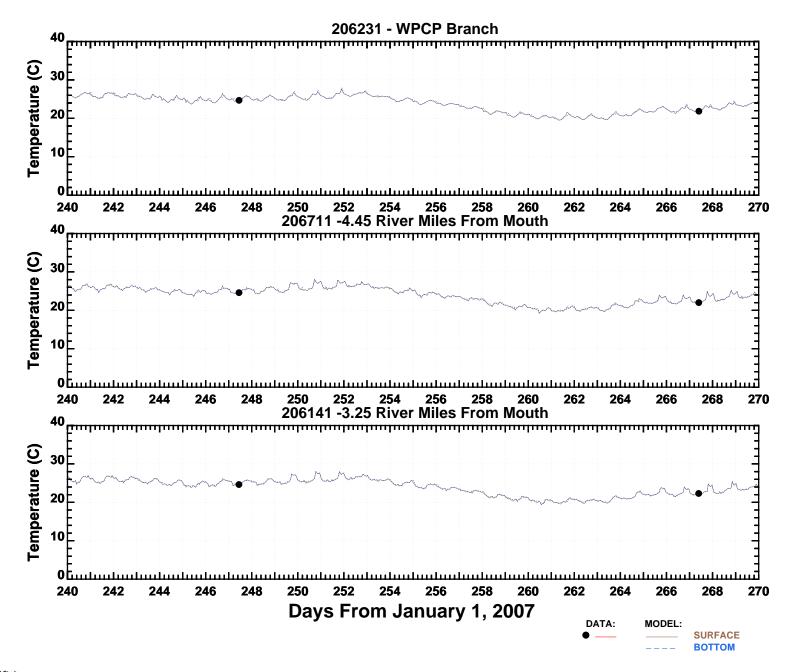


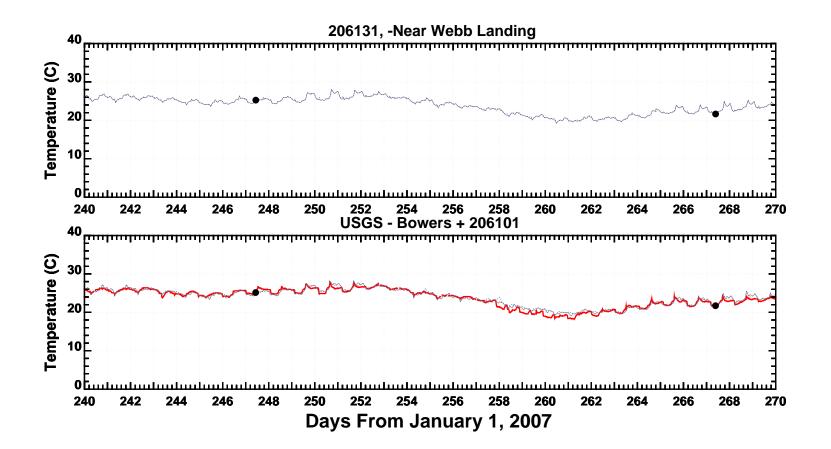


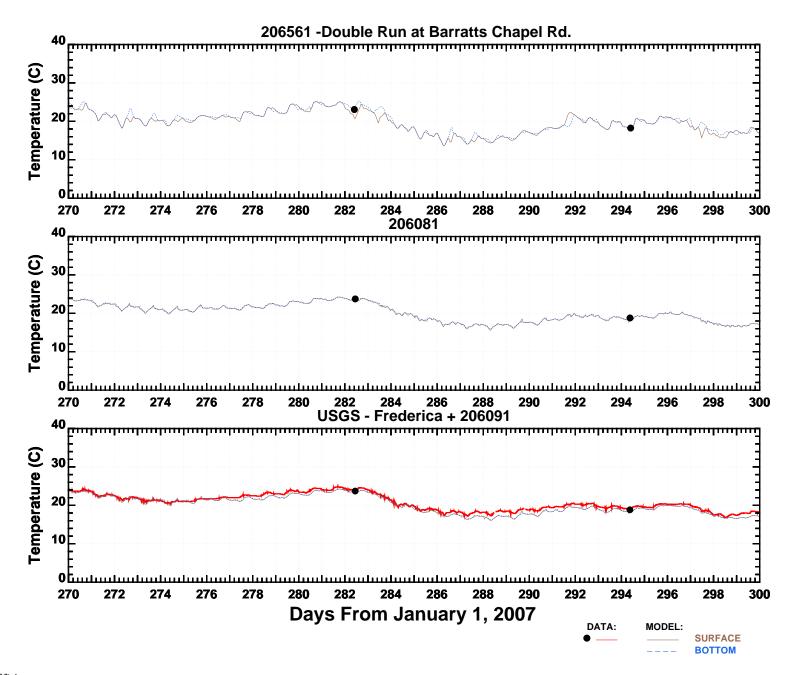


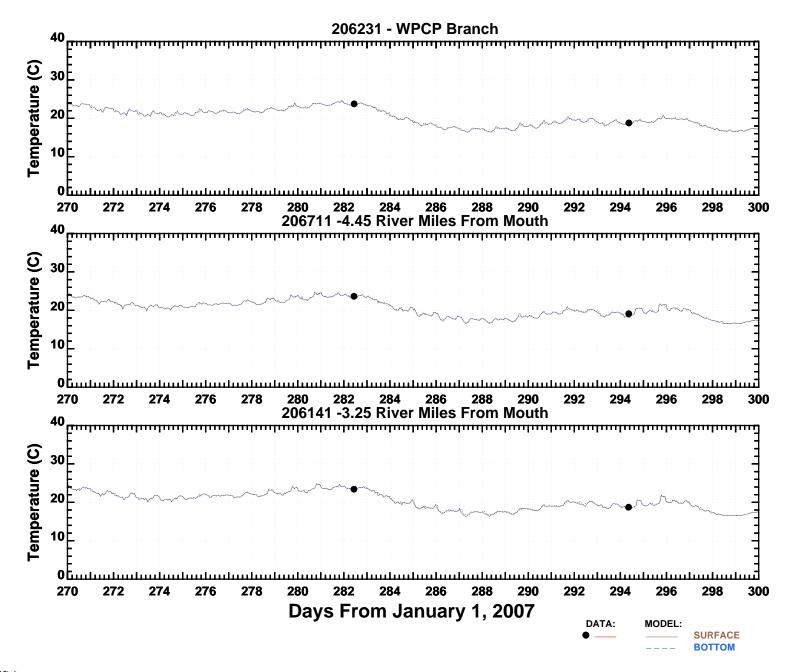


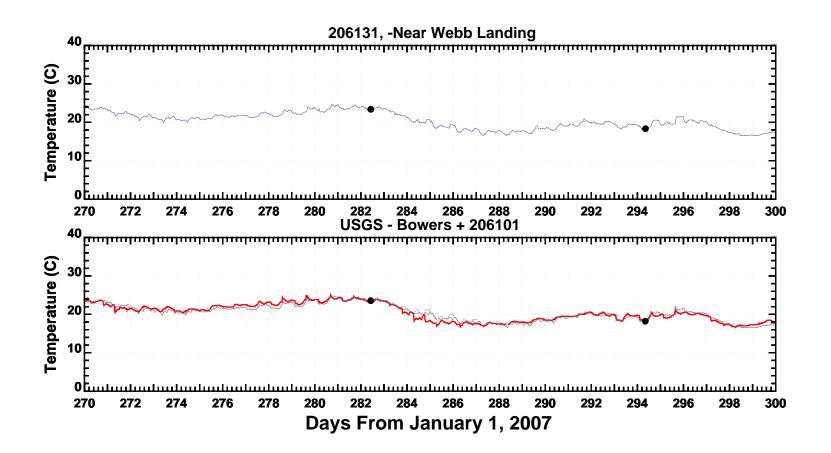






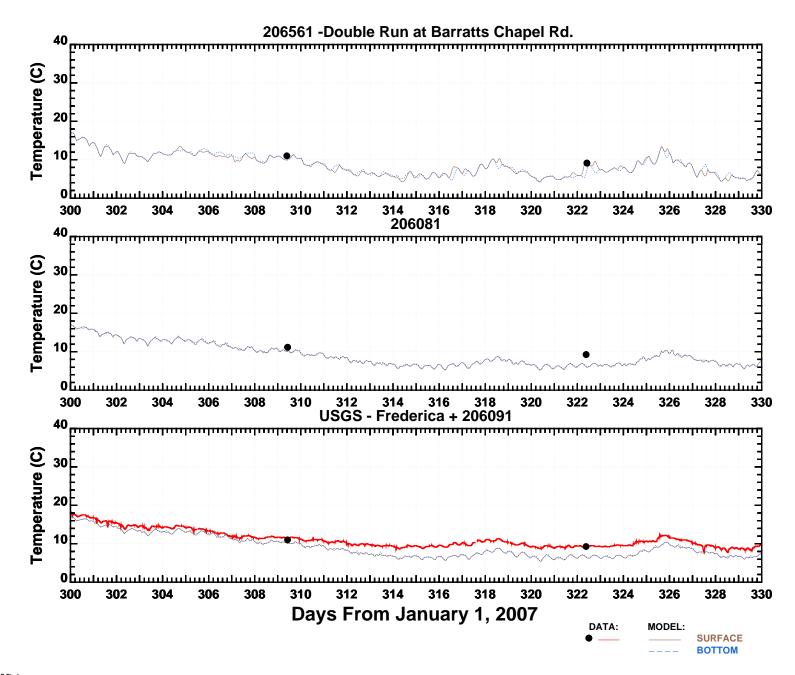


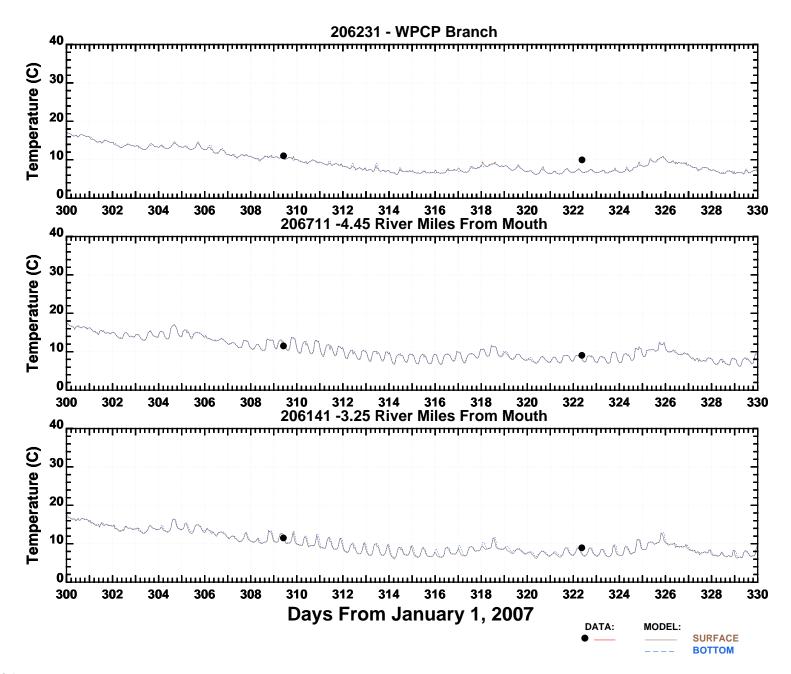


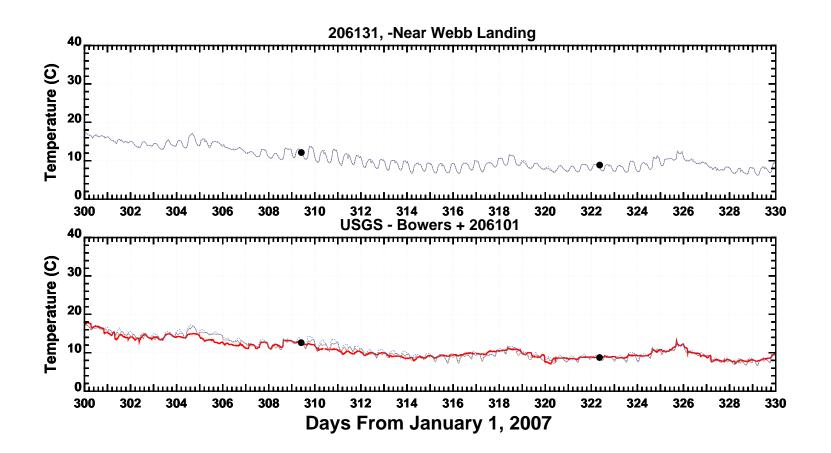


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BOTTOM

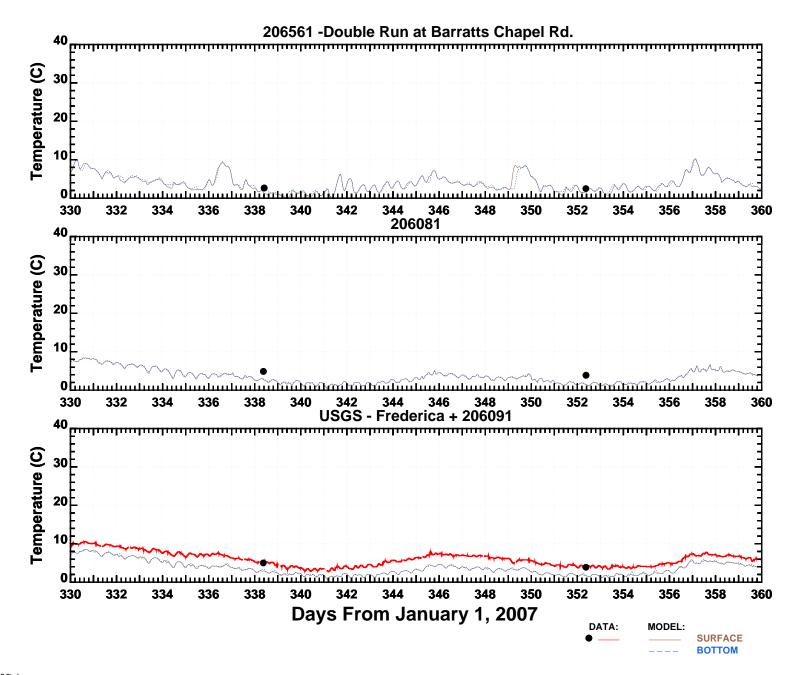


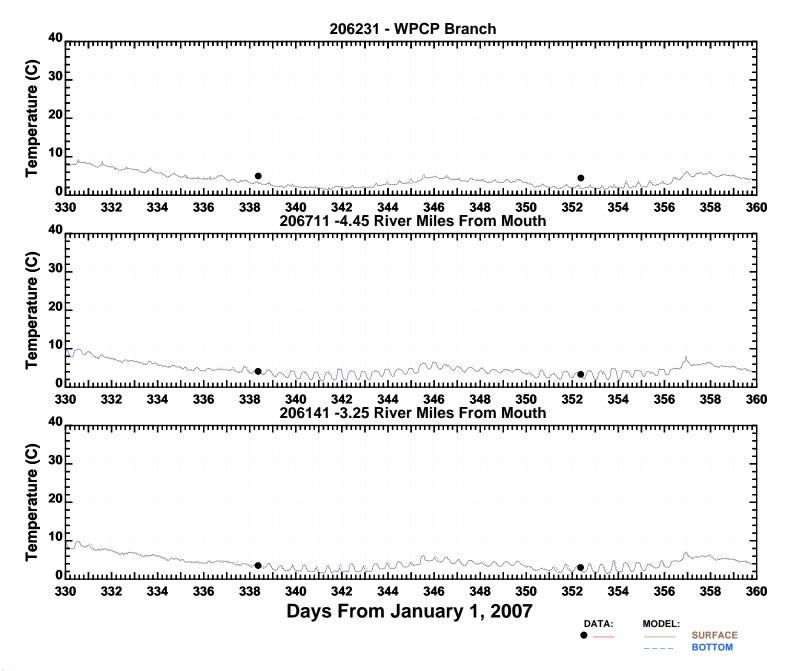


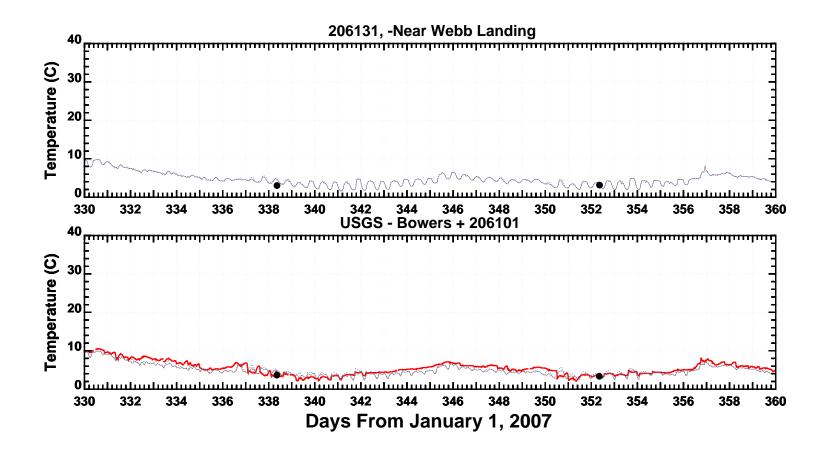


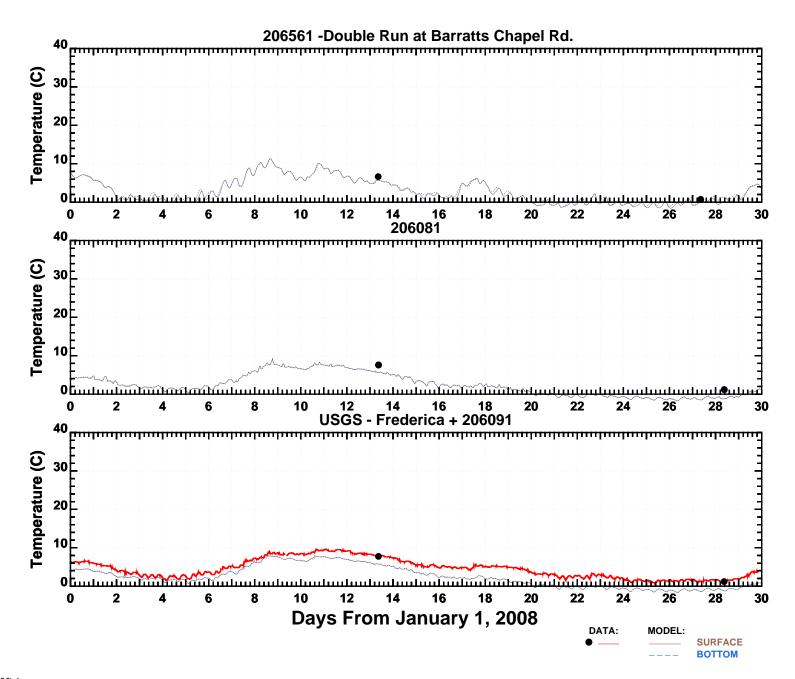
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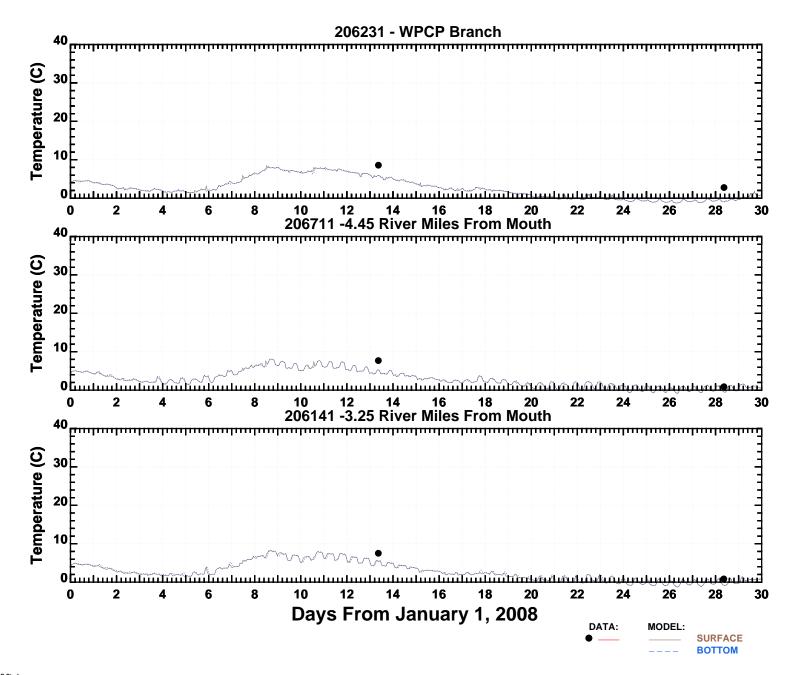
SURFACE
BOTTOM

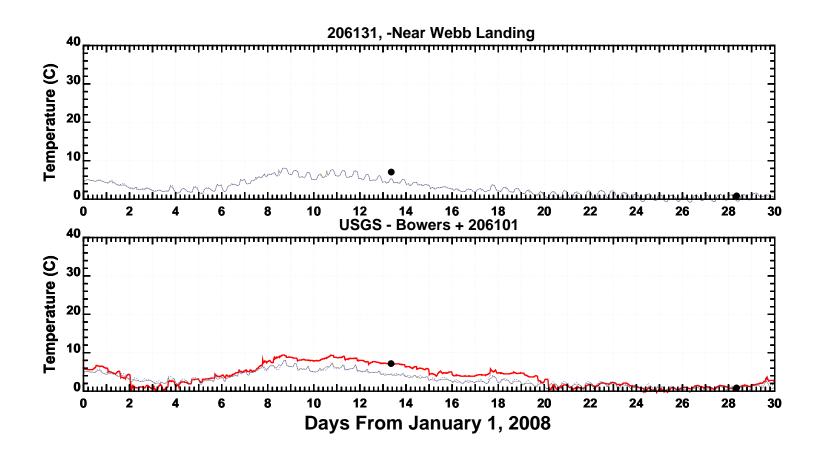


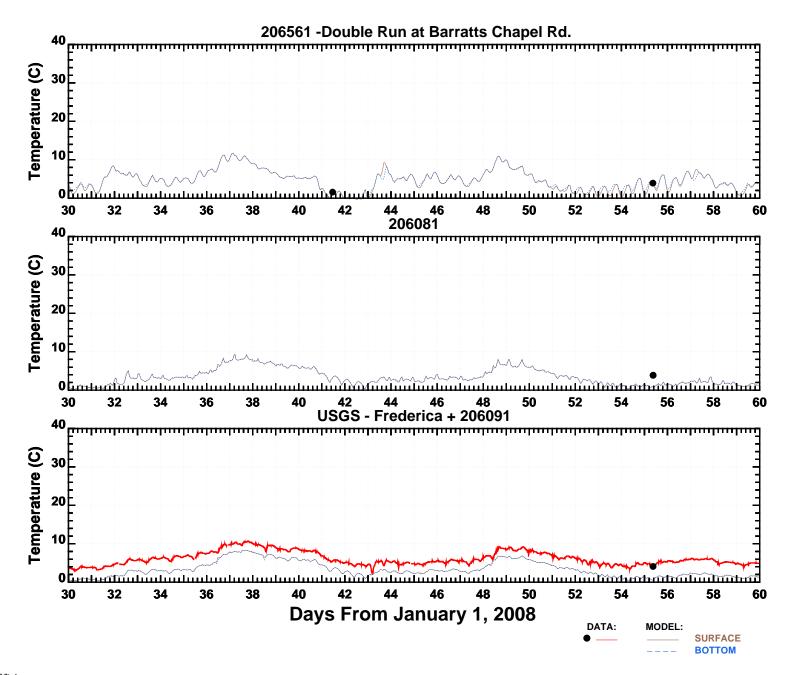


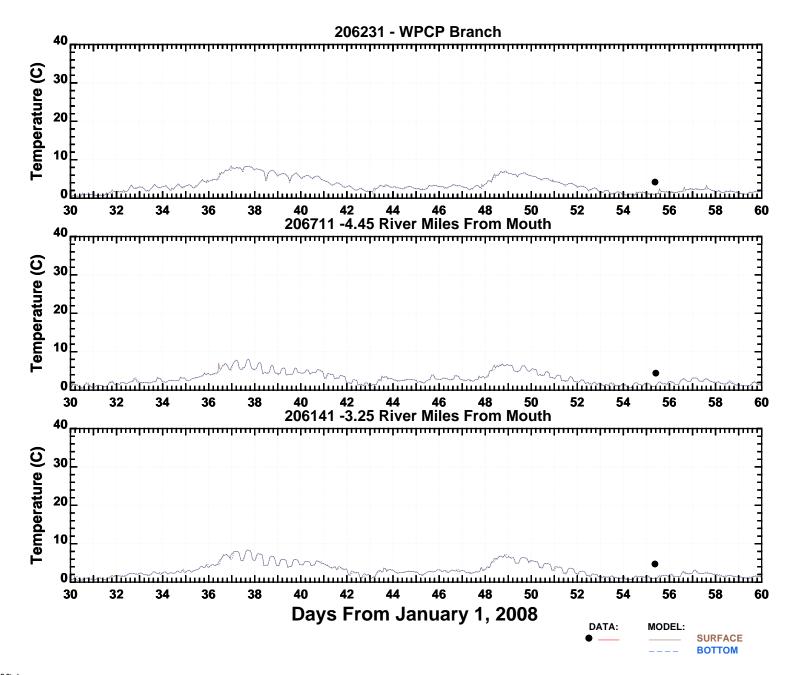


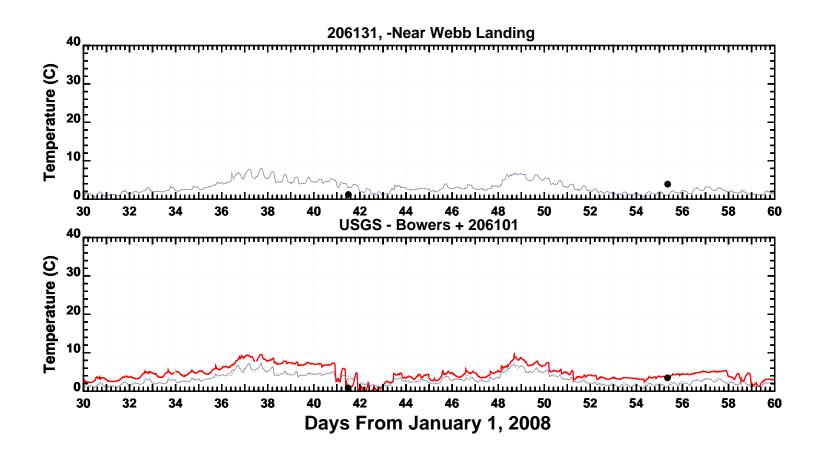


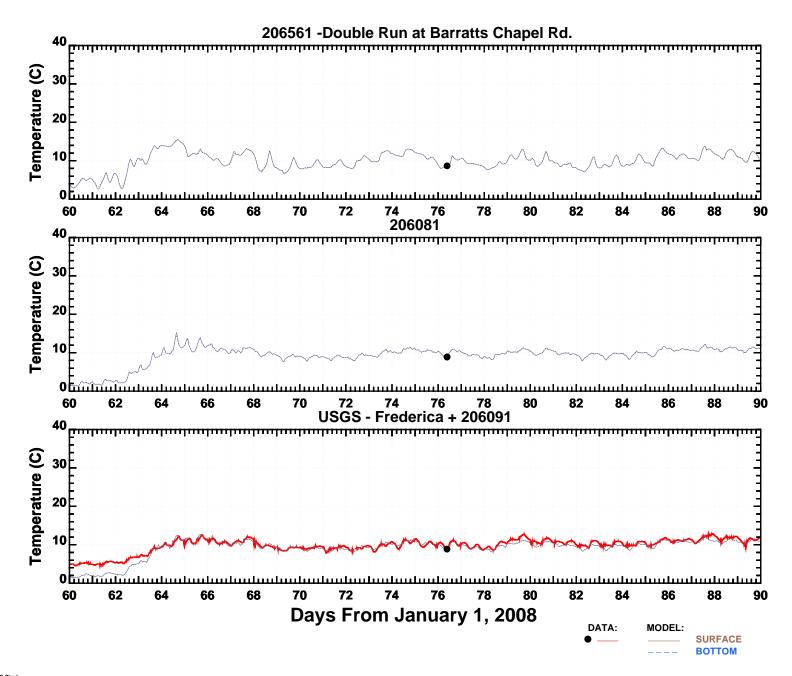


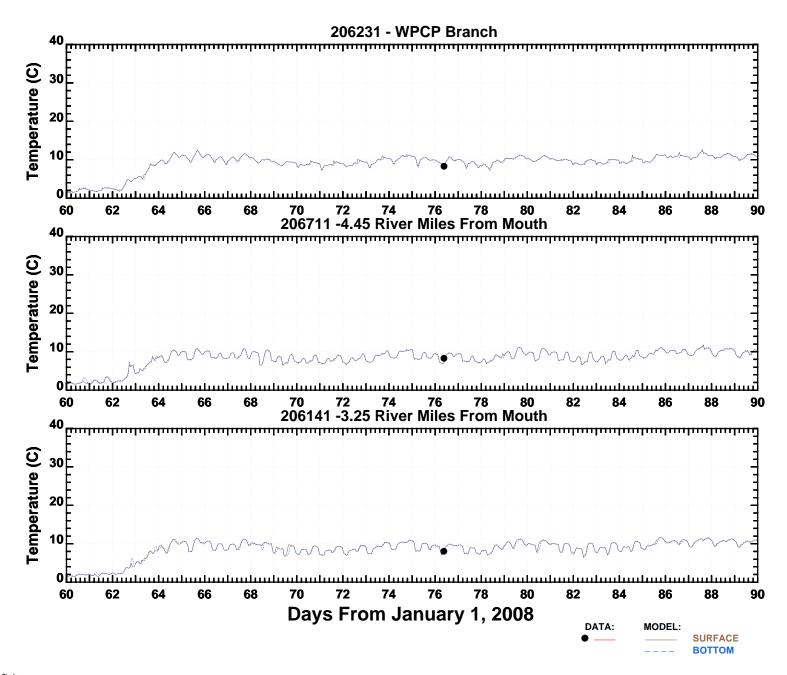


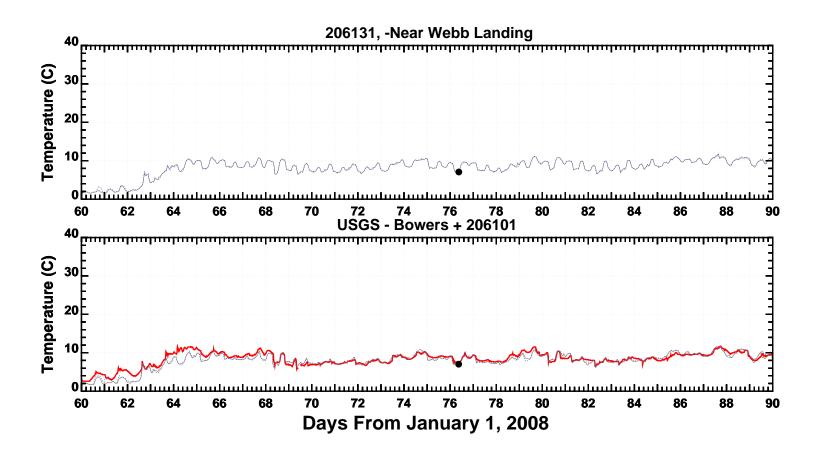


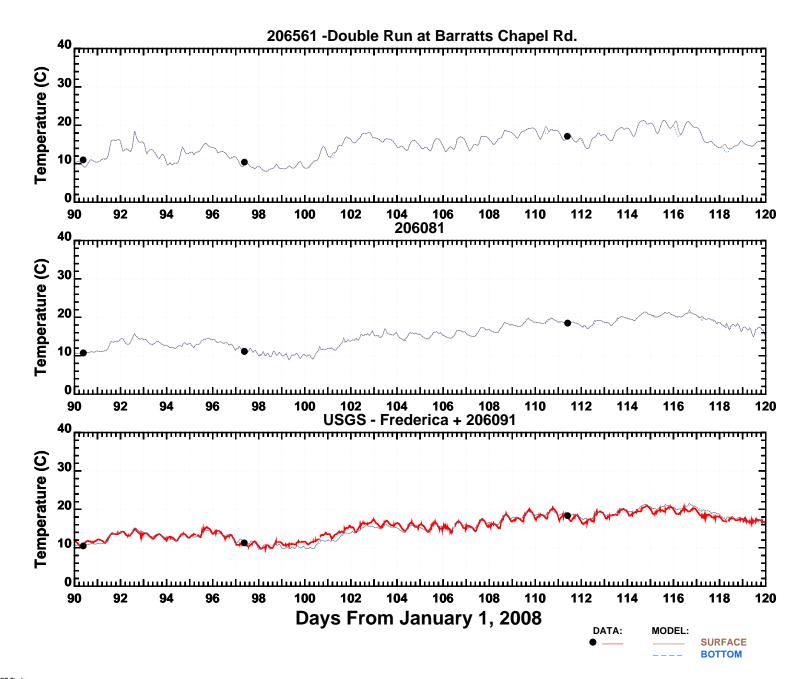


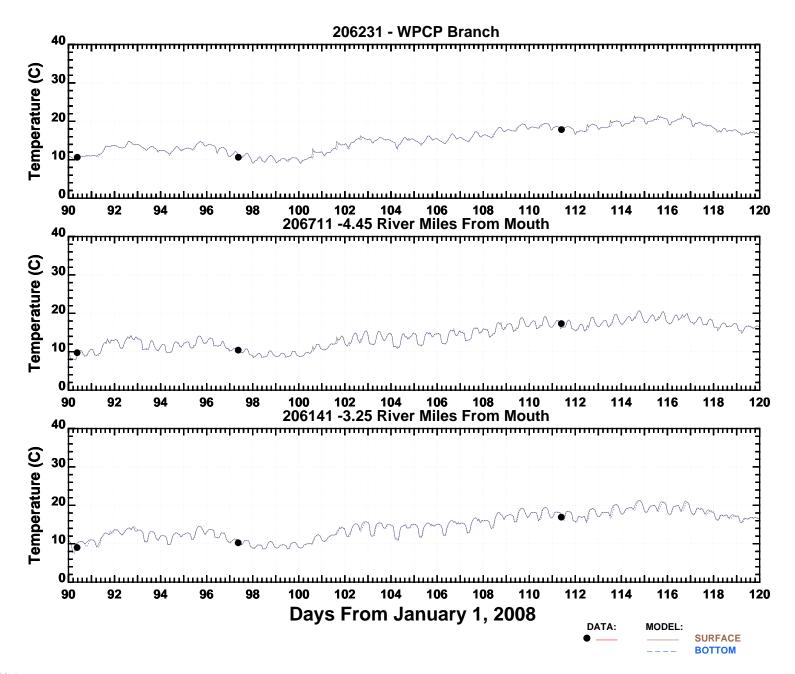










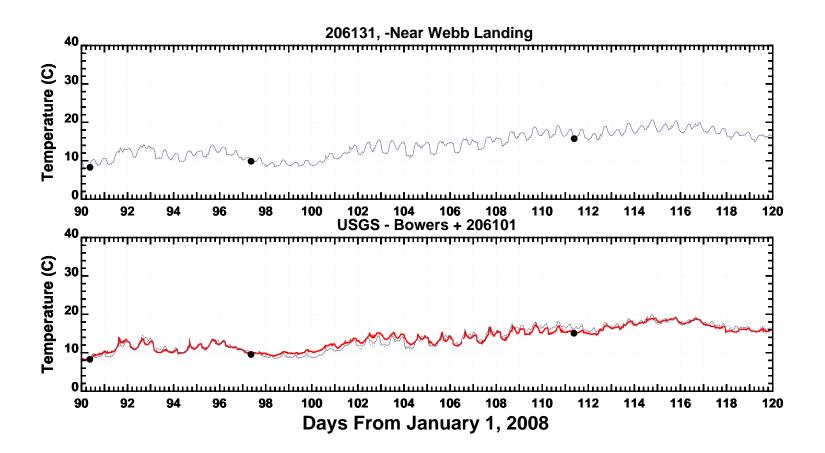


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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows



DATA: MODEL:

● \_\_\_\_ SURFACE

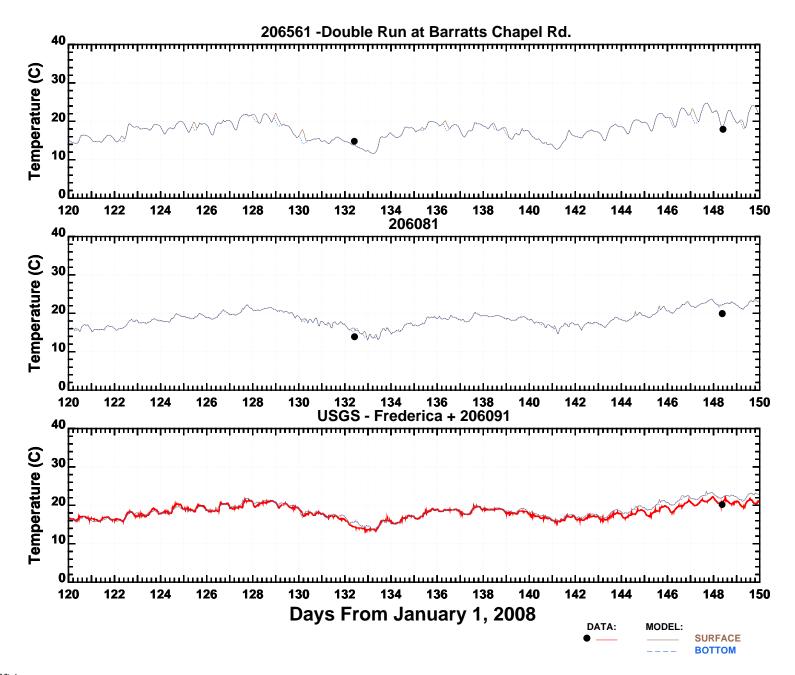
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DNREC Study

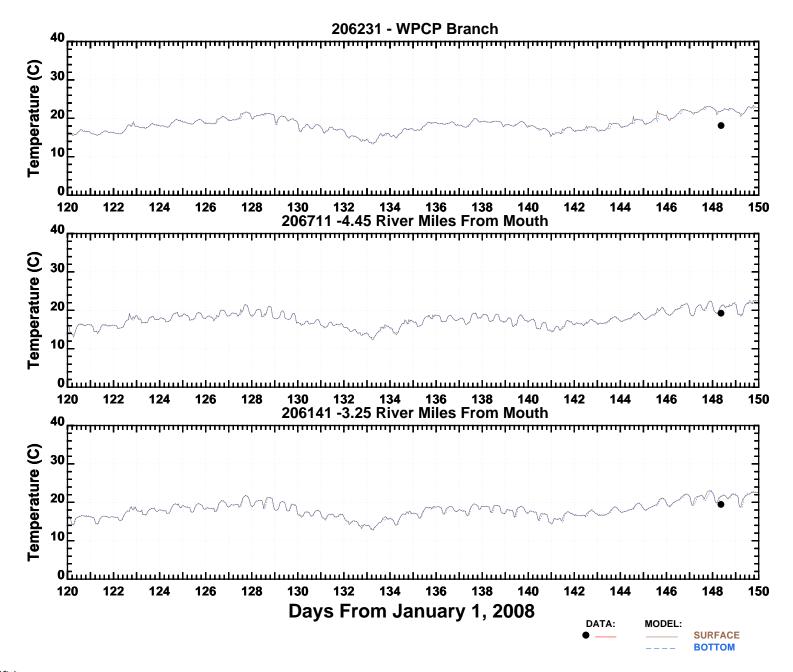
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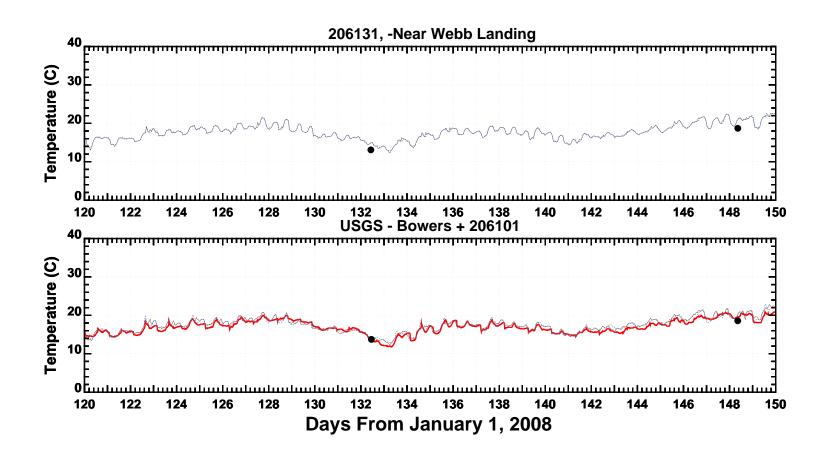
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DNREC Study
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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows .



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/birchi/kcdw0014/HYDRO/PLOTS/TANDS/tempReport.gdp
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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows



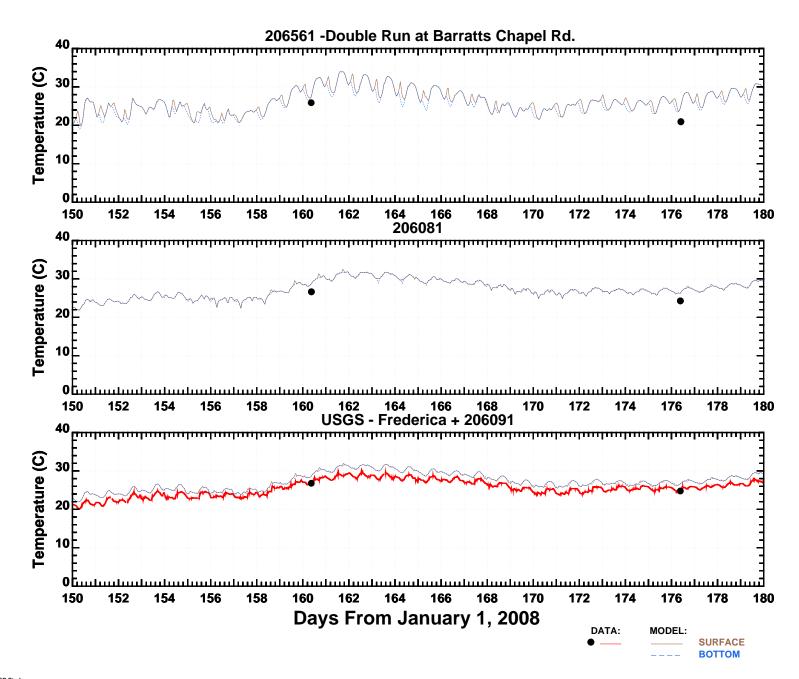


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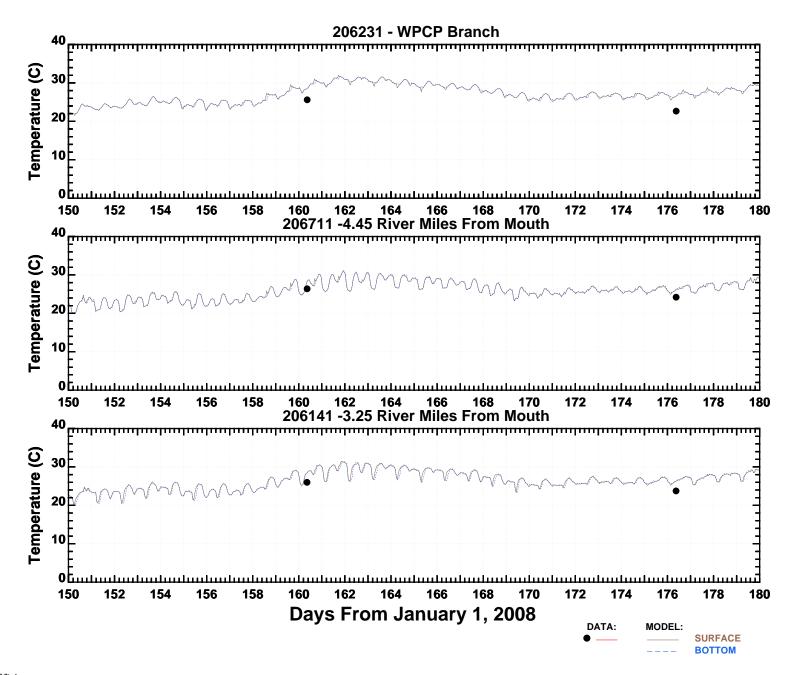
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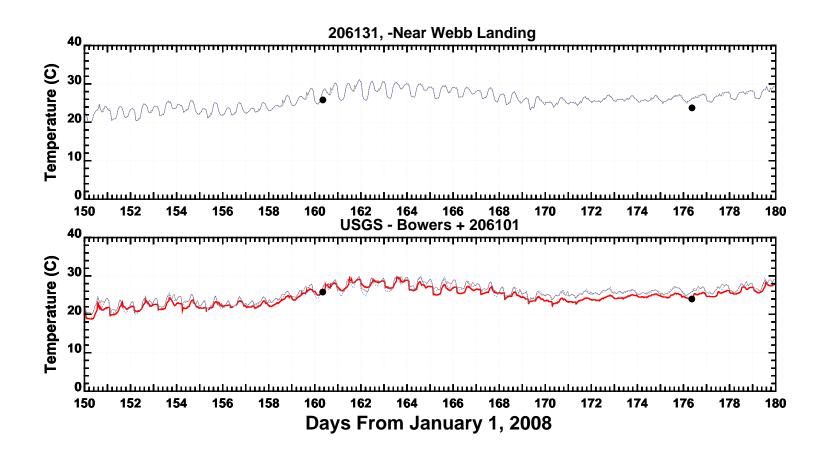
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DNREC Study
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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows .



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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows



DATA: MODEL:

■ \_\_\_\_ SURFACE

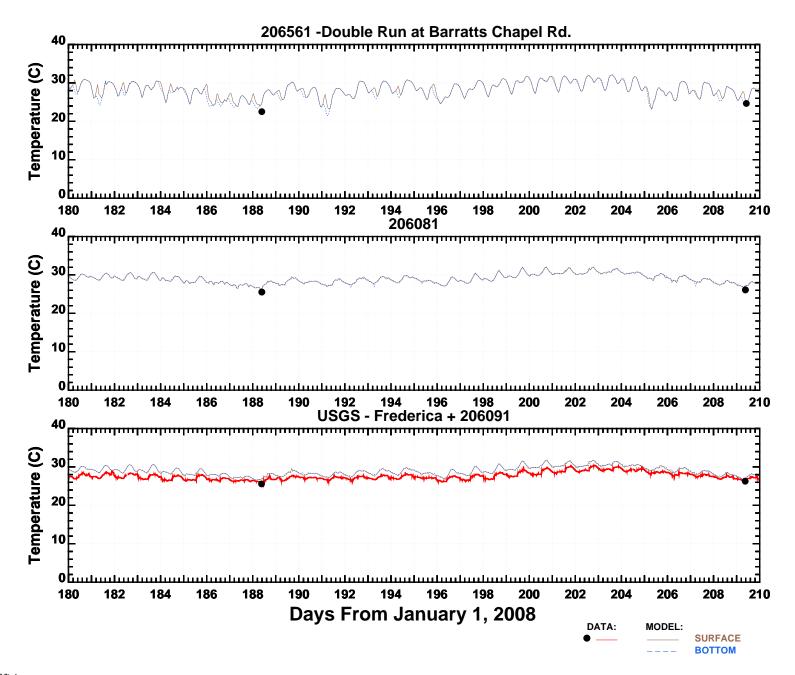
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DNREC Study

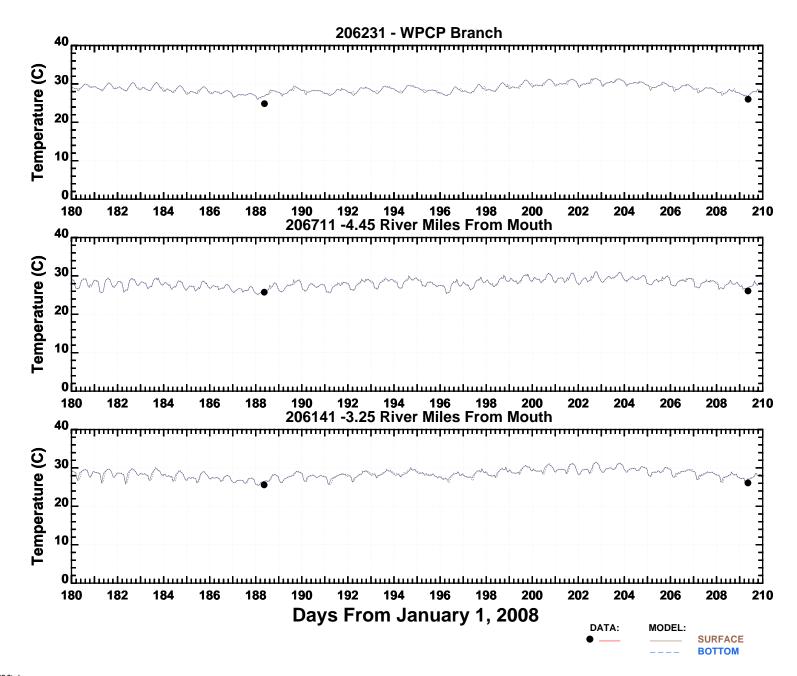
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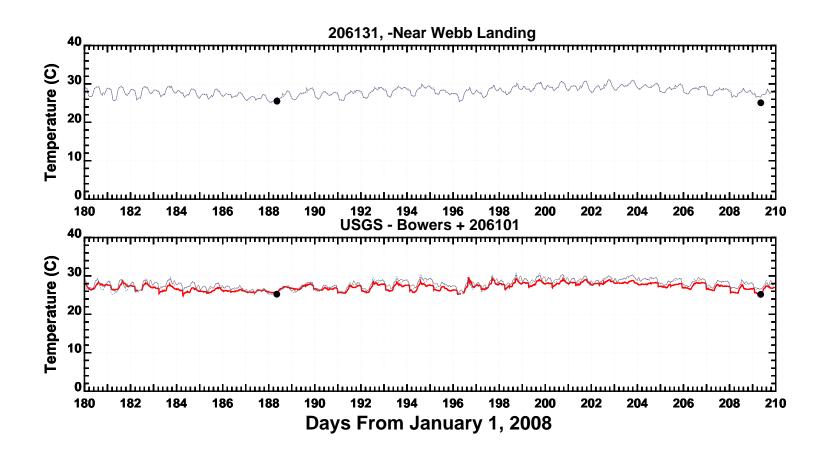
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DNREC Study
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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows



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/birchi/kcdw0014/HYDRO/PLOTS/TANDS/tempReport.gdp
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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows



DATA: MODEL:

■ \_\_\_\_ SURFACE

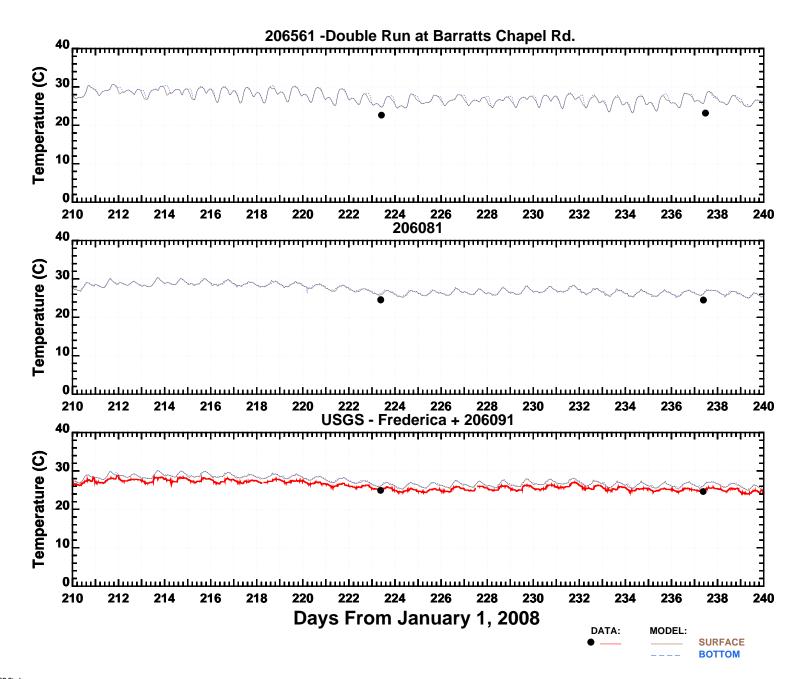
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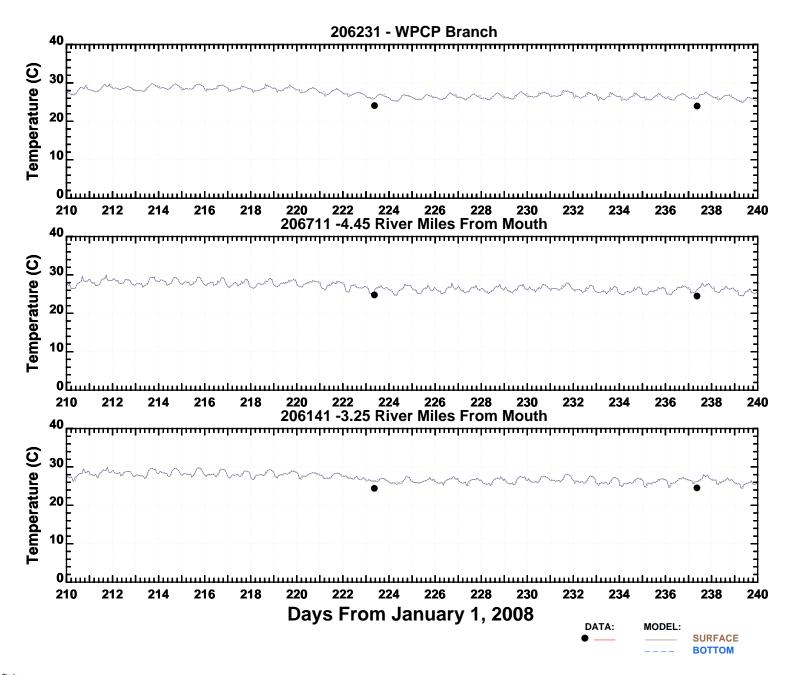
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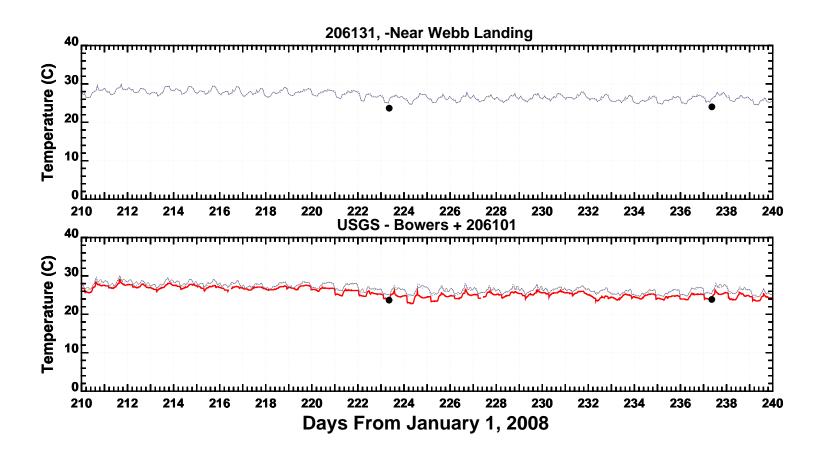
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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows



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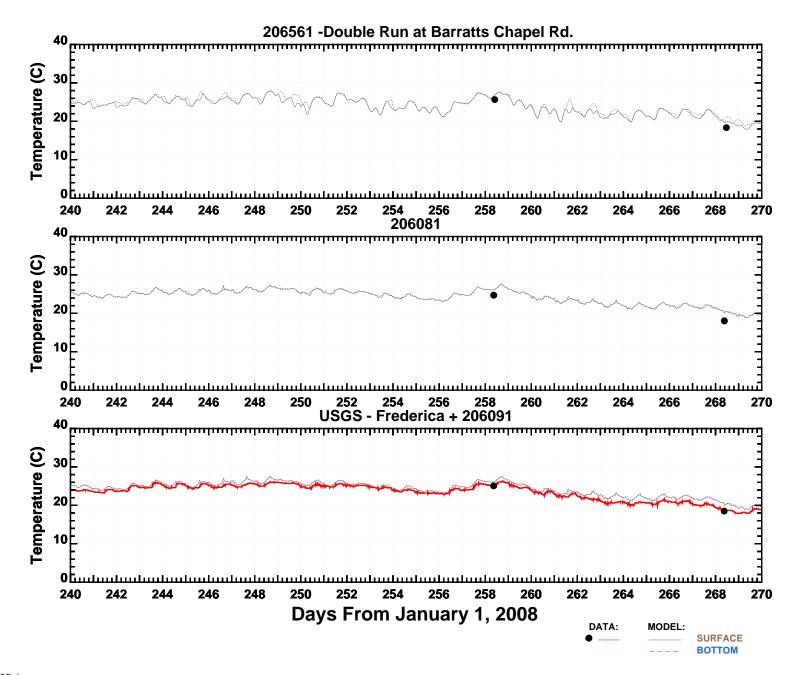
■ \_\_\_\_ SURFACE
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DNREC Study

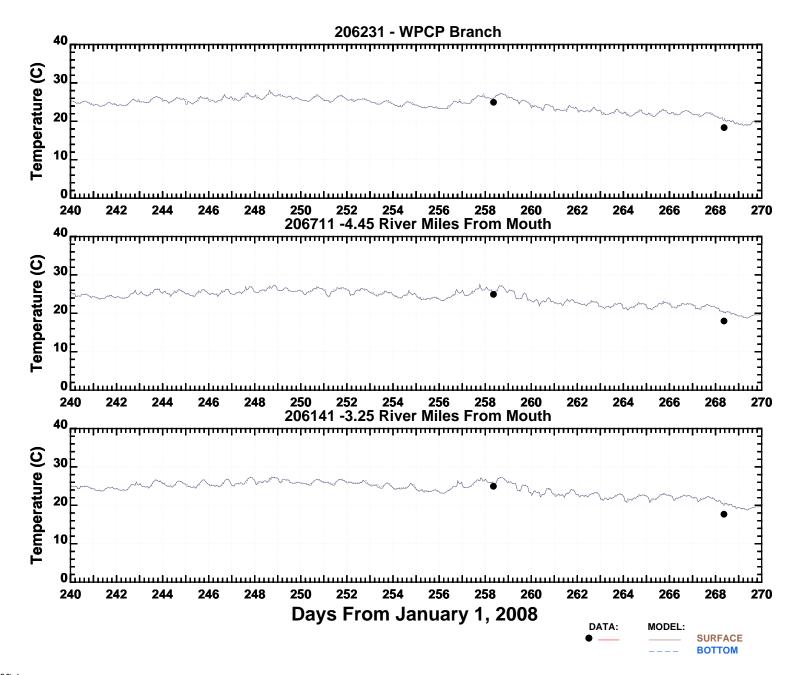
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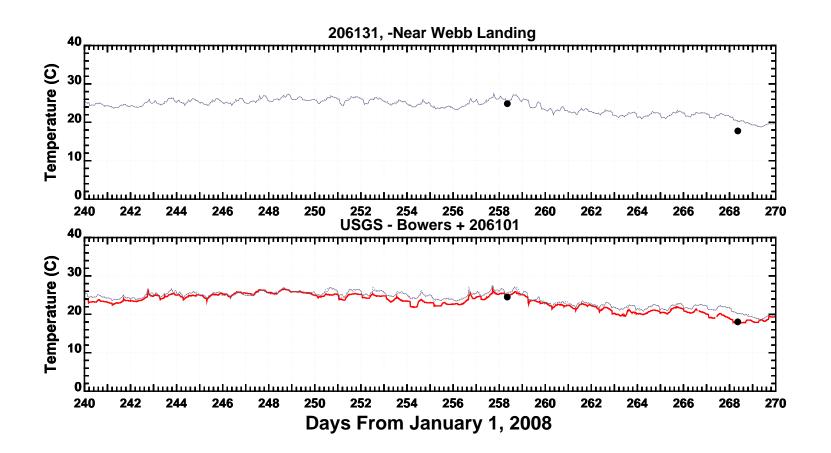
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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows



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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows



DATA: MODEL:

■ \_\_\_\_ SURFACE

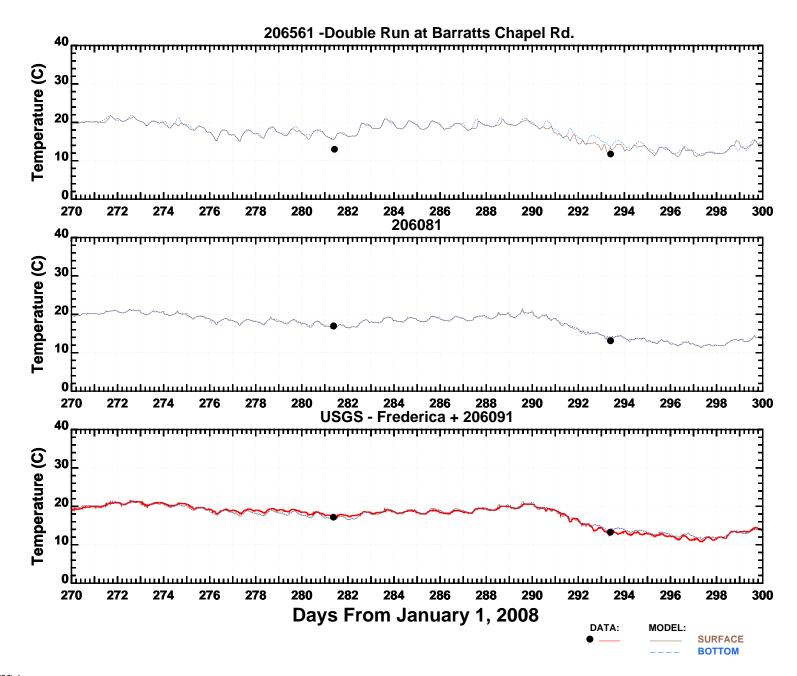
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DNREC Study

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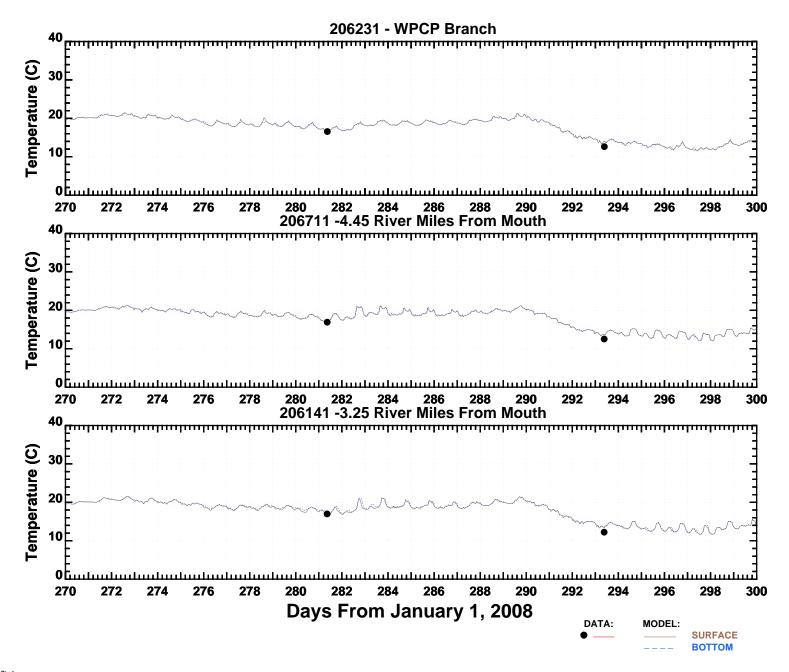


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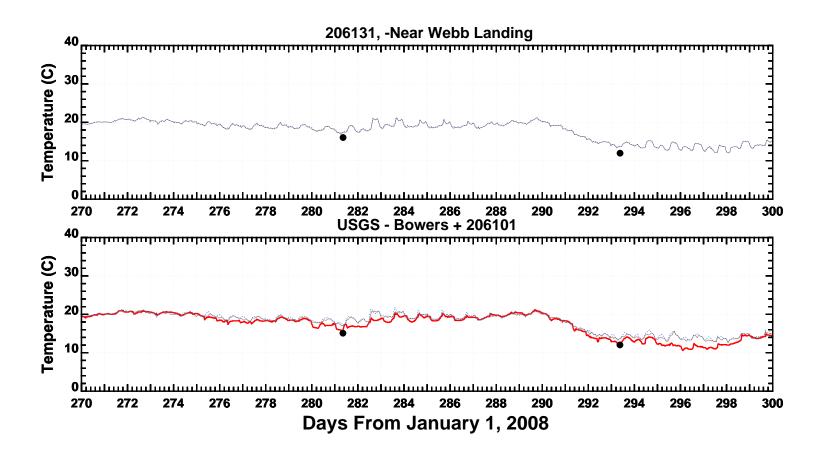
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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows



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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows



DATA: MODEL:

■ \_\_\_\_ SURFACE

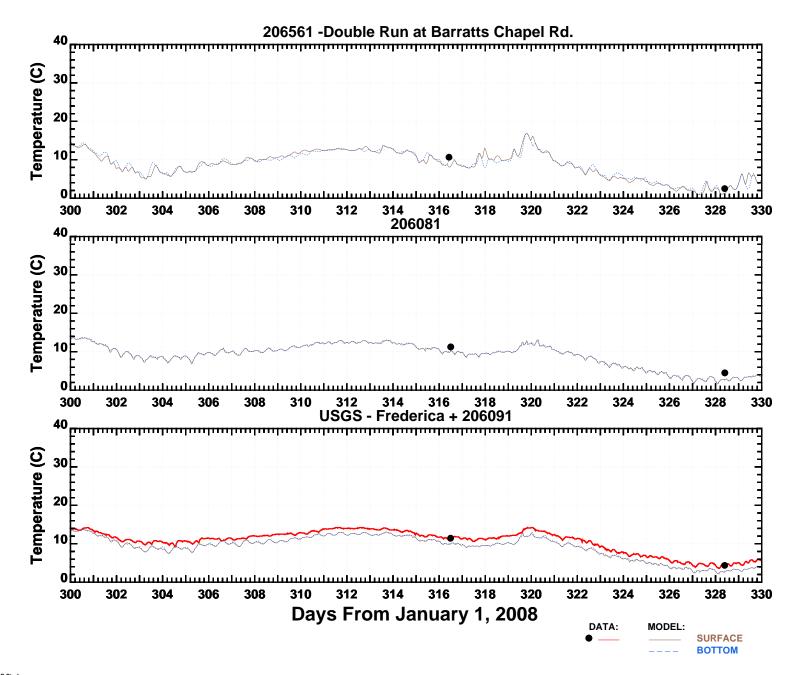
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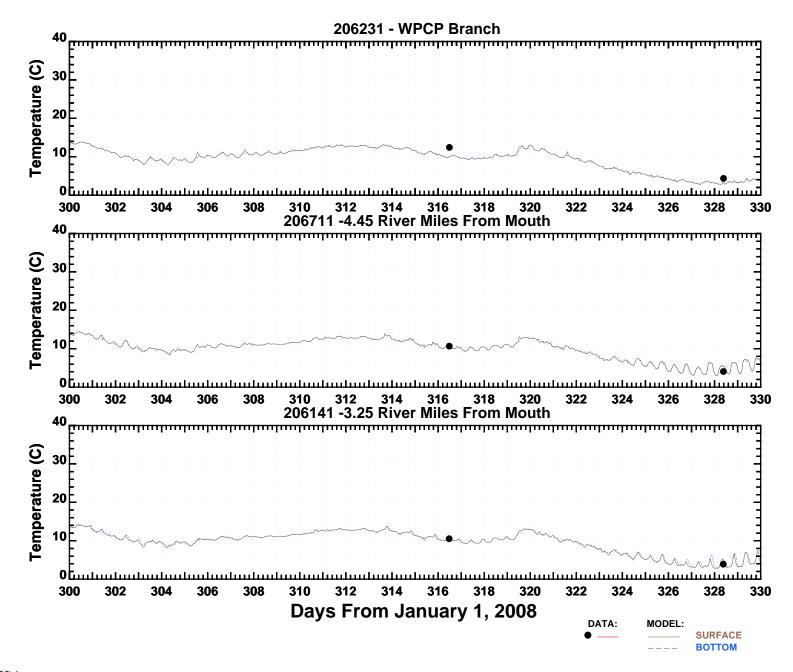


DNREC Study

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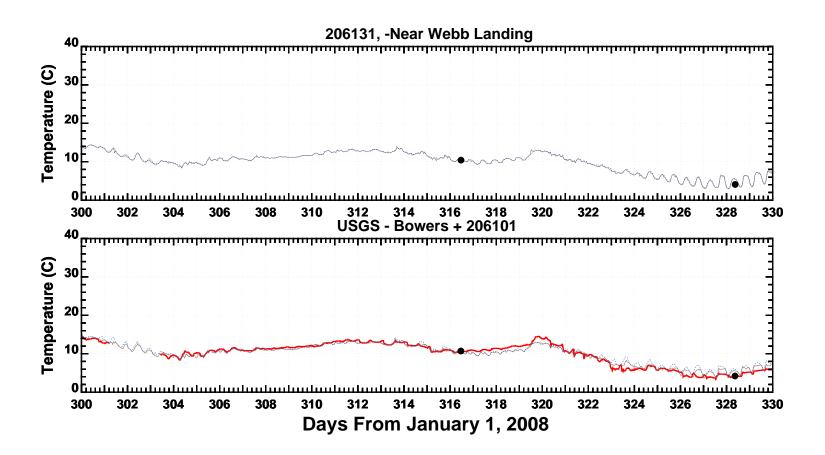


DNREC Study

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■ \_\_\_\_ SURFACE

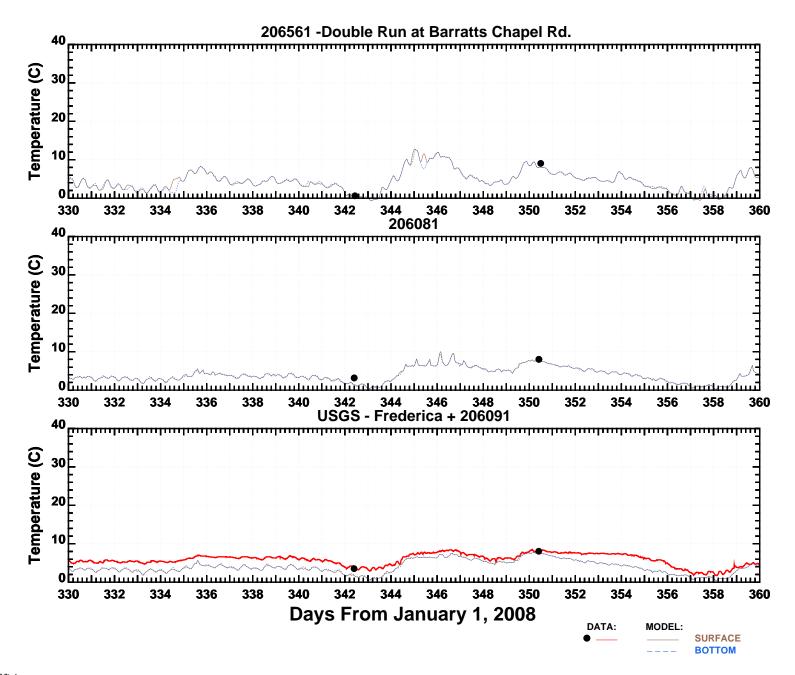
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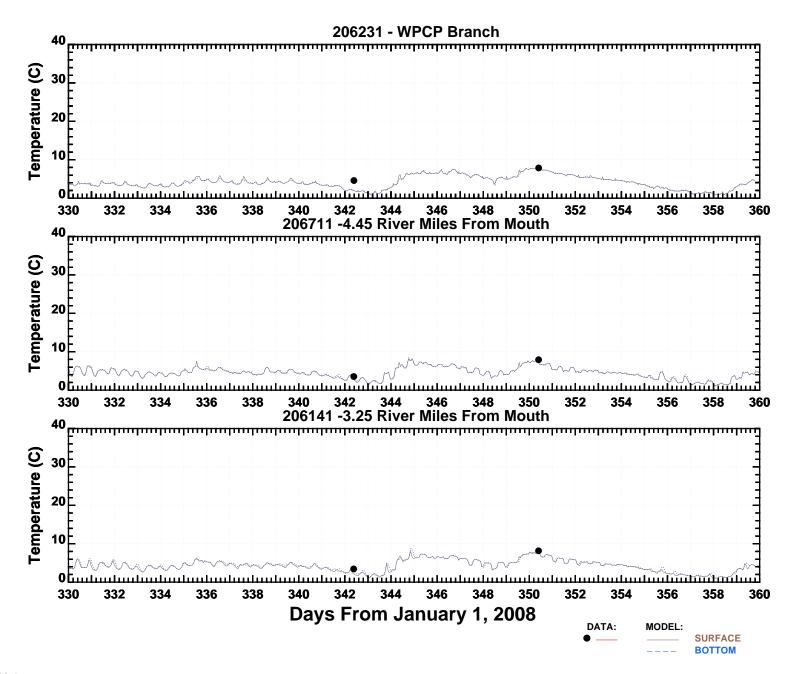
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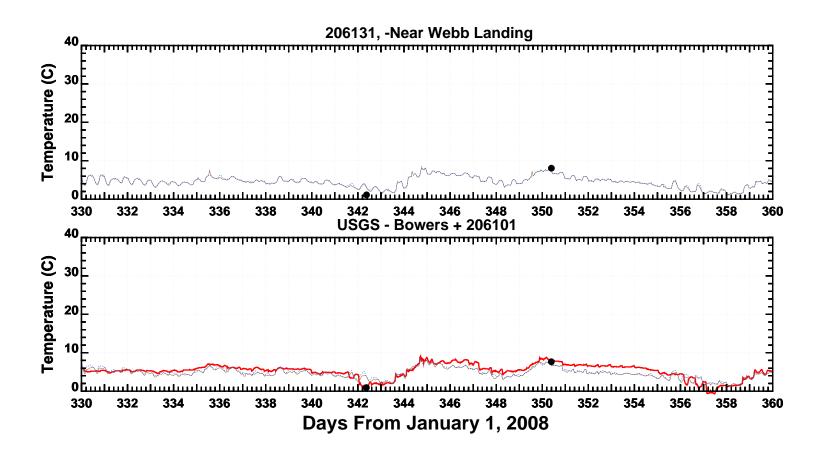
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DNREC Study
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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows .



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/birchi/kcdw0014/HYDRO/PLOTS/TANDS/tempReport.gdp
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08RUN003: 010708\*v18.thindams,defaultBFRIC,HORCONx0.1, BowersDailyAvesalt-stratified-3,New100% flows .



DATA: MODEL:

■ \_\_\_\_ SURFACE

--- BOTTOM

DNREC Study

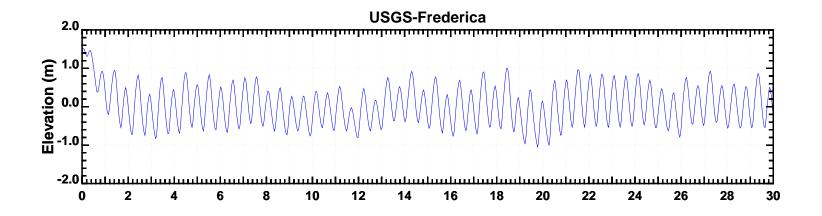
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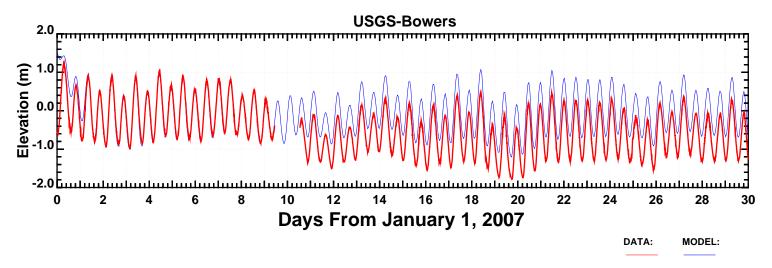
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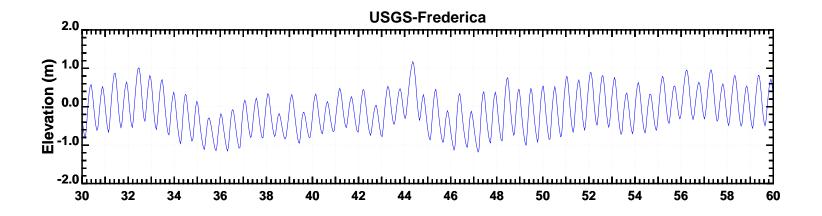
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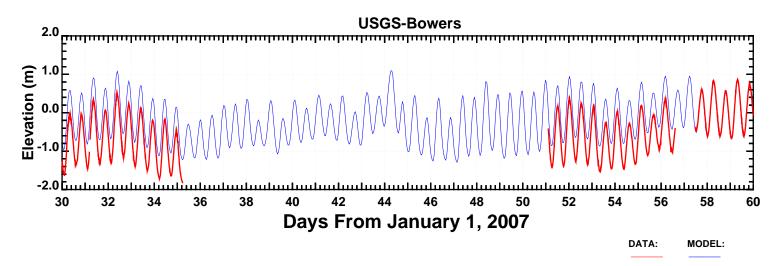
## **APPENDIX 5**

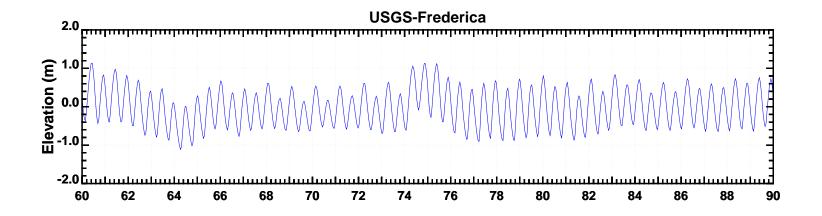
## HYDRODYNAMIC MODEL WATER ELEVATION CALIBRATION/VALIDATION FIGURES

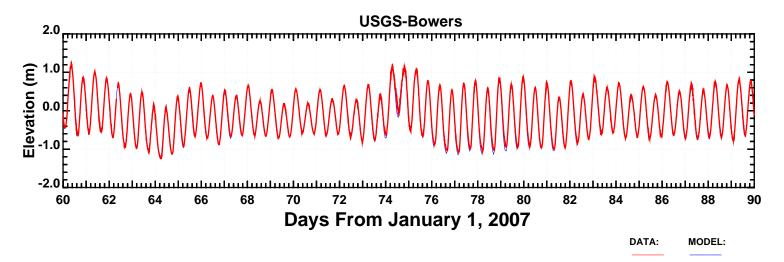


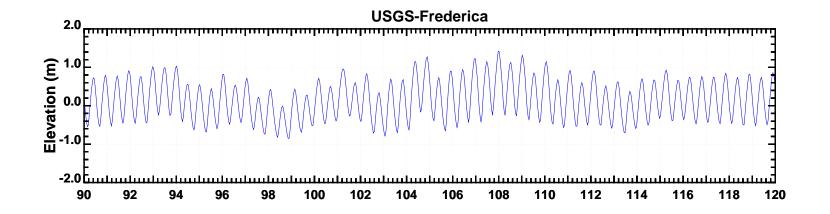


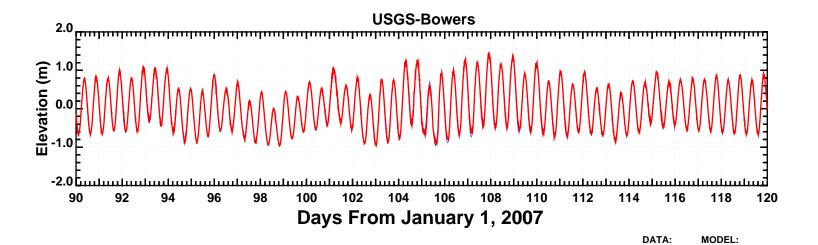


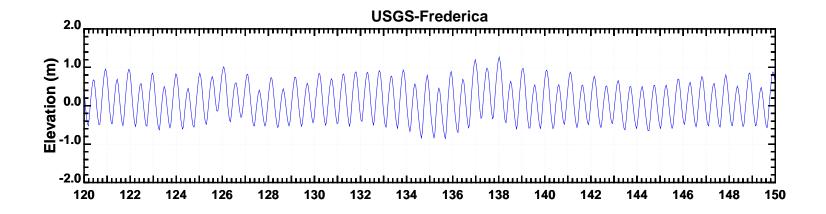


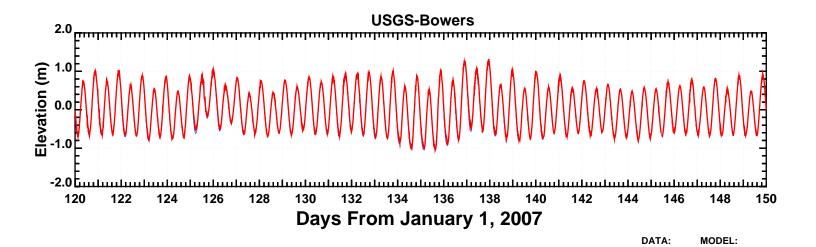




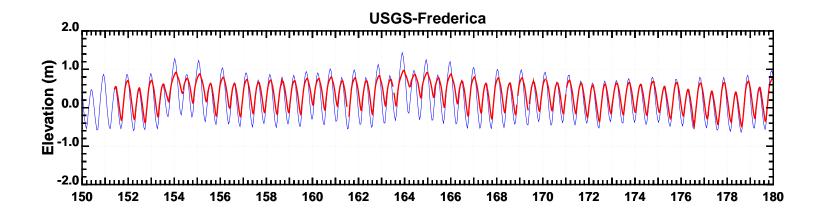


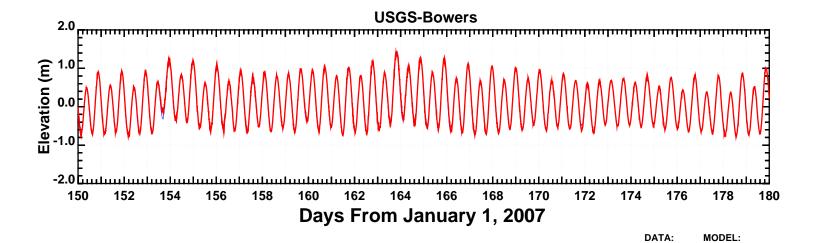




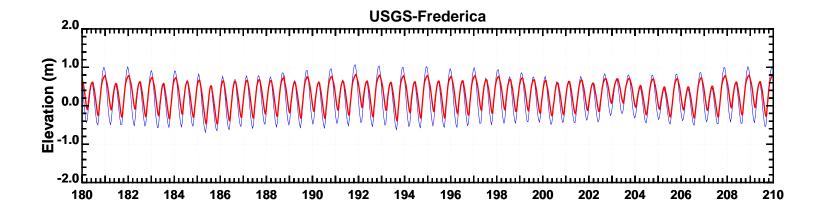


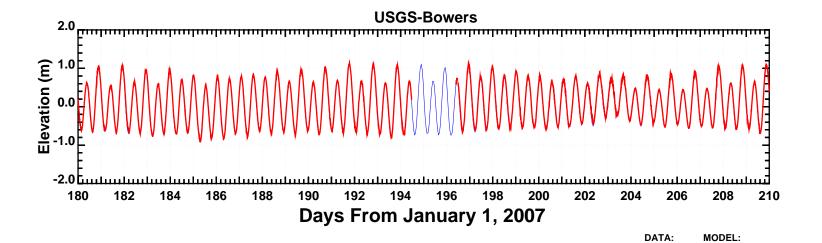
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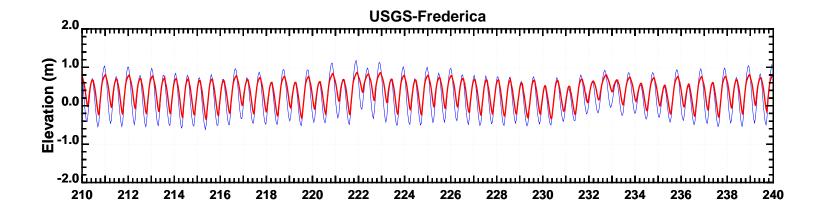


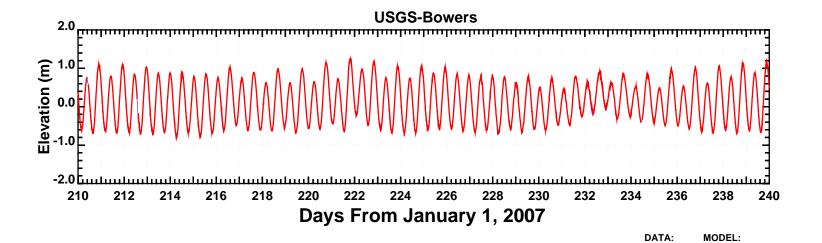
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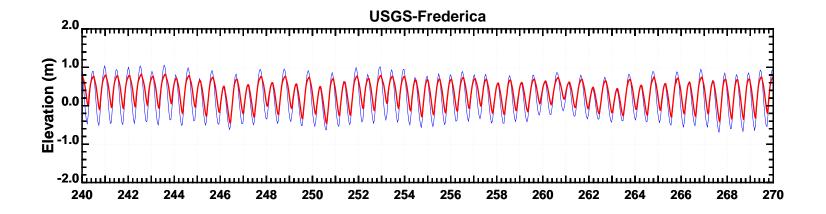


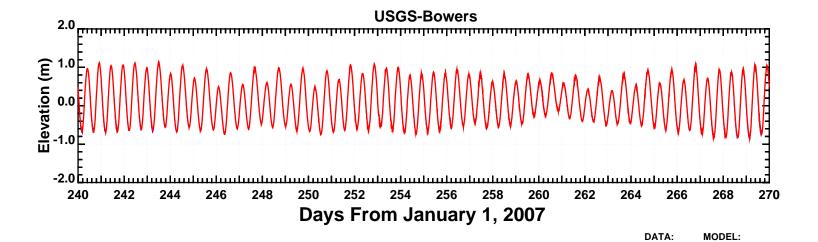
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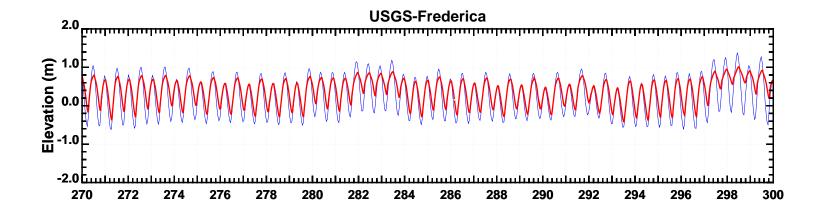


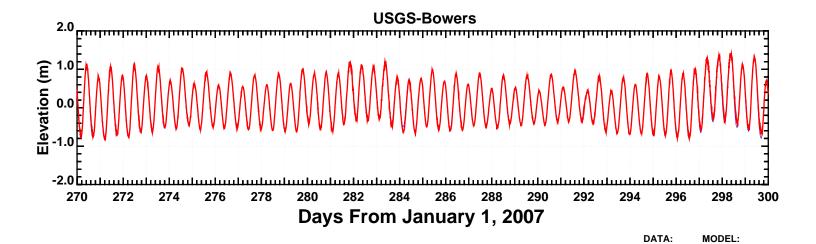


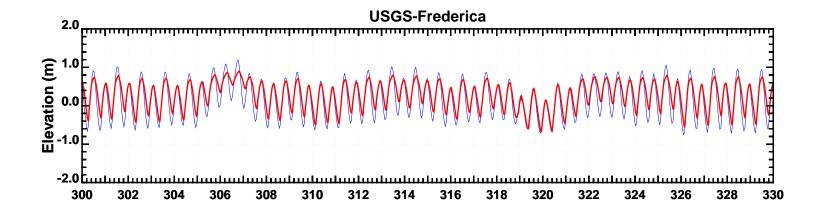
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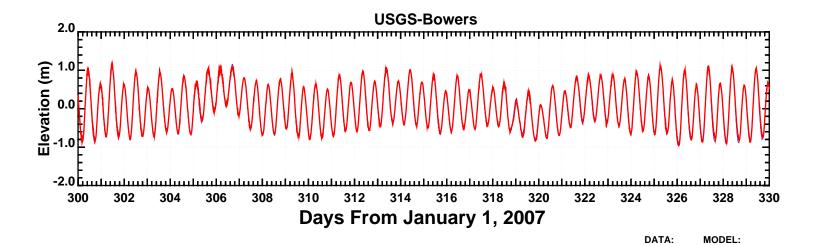


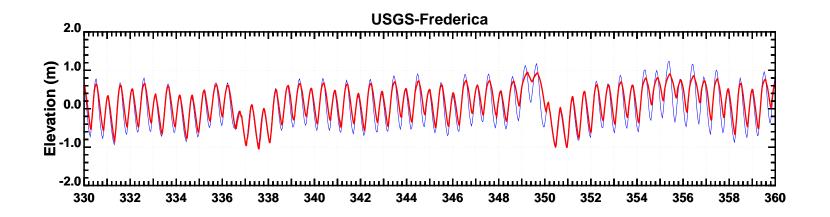


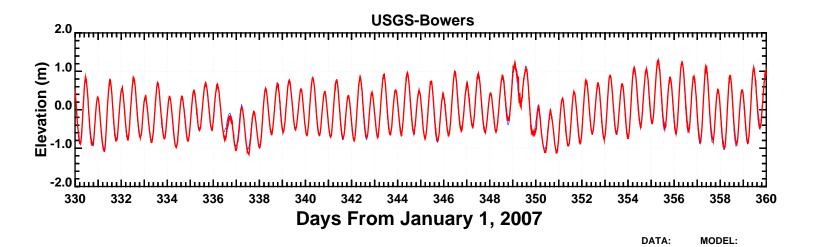




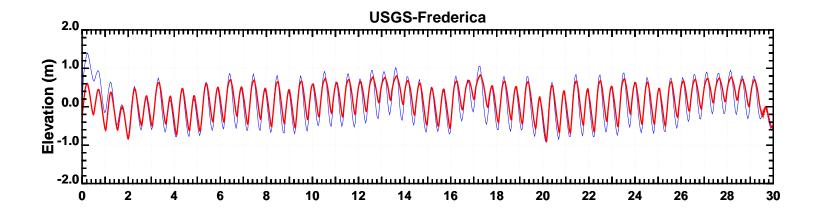


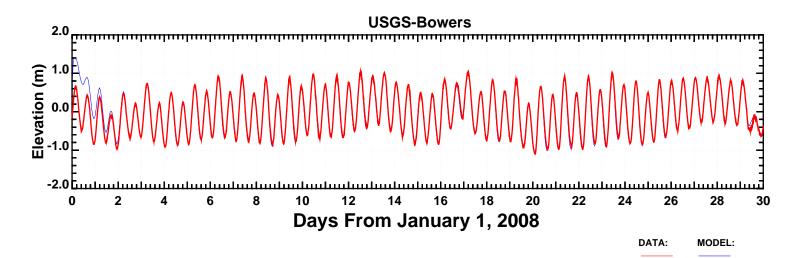


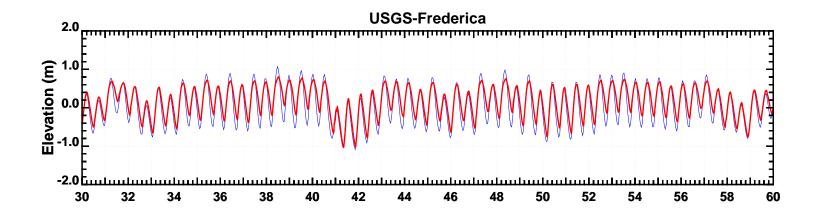


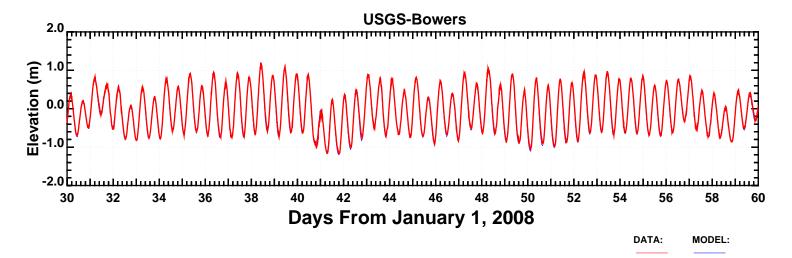


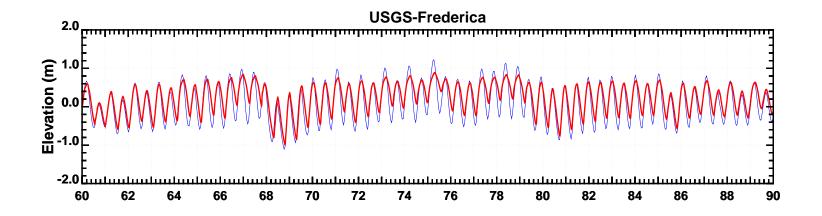
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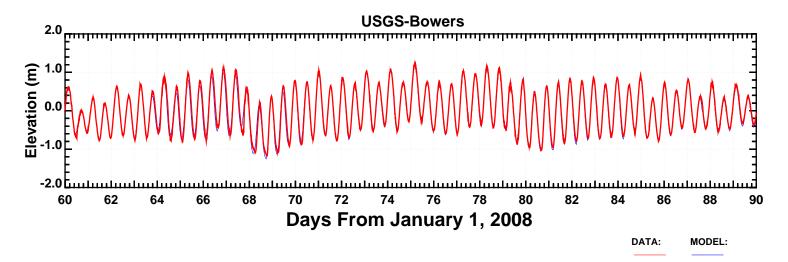


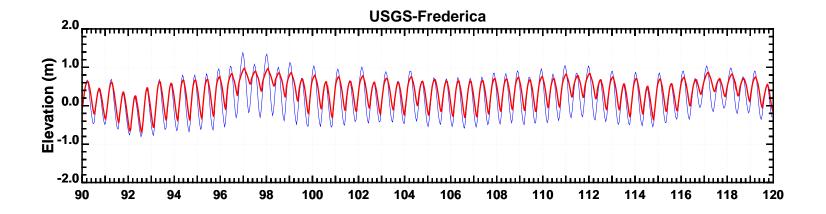


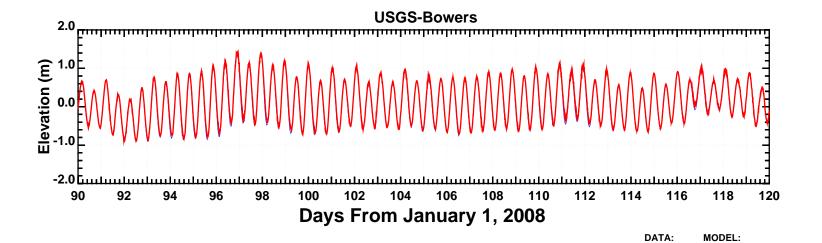




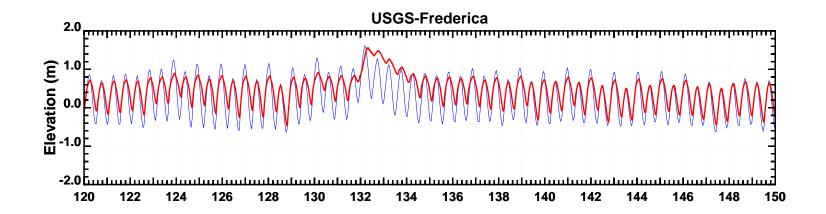


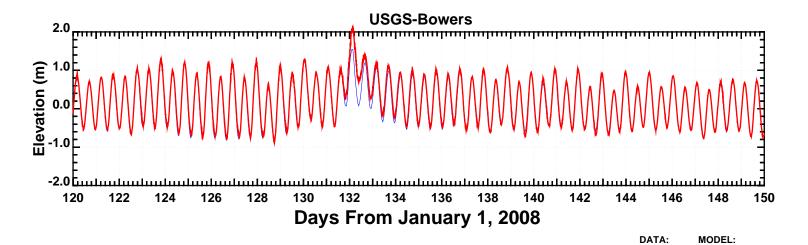




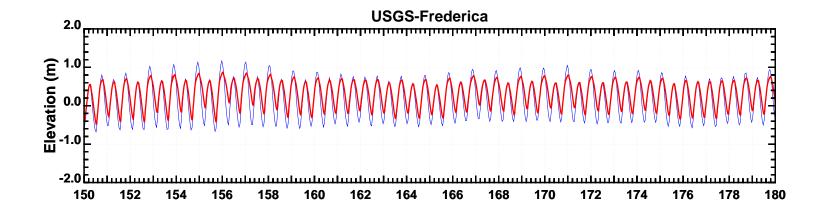


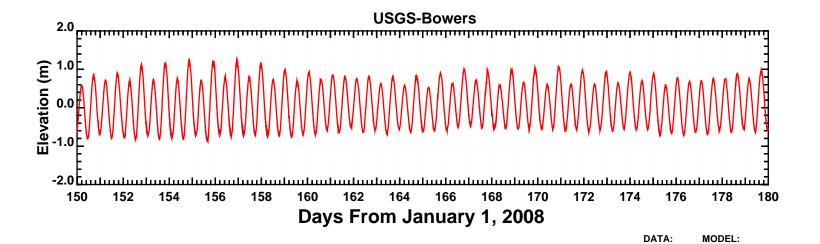
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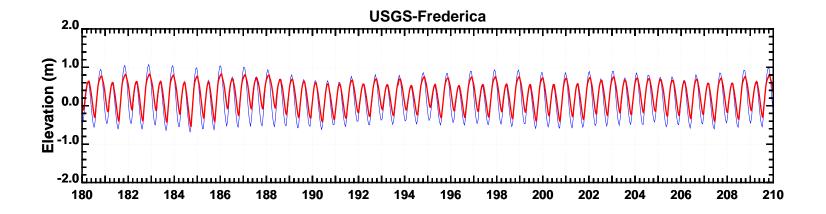


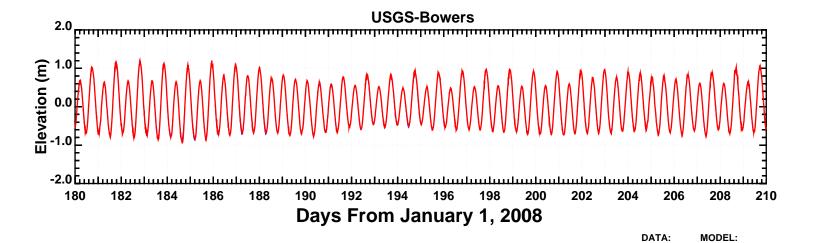


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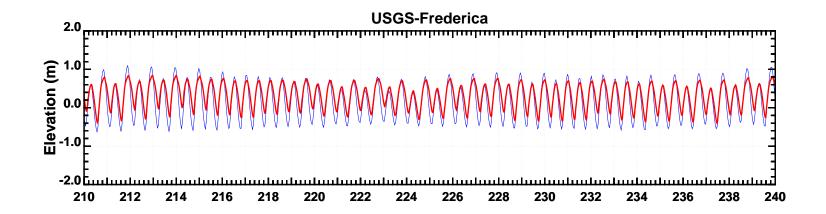


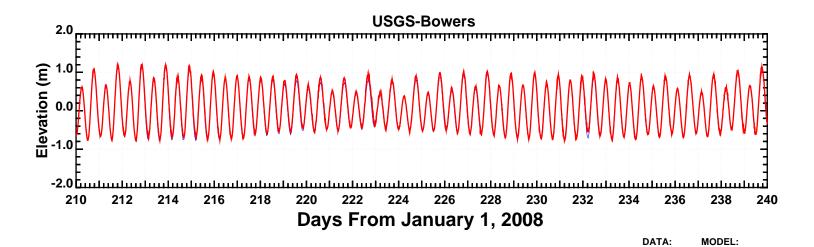




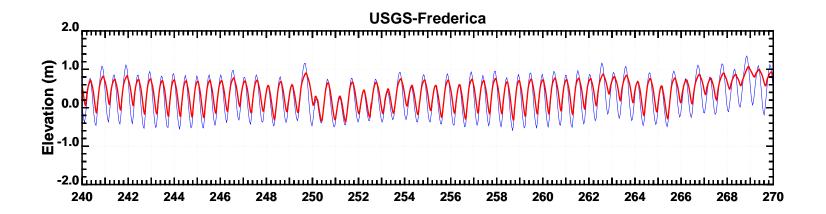


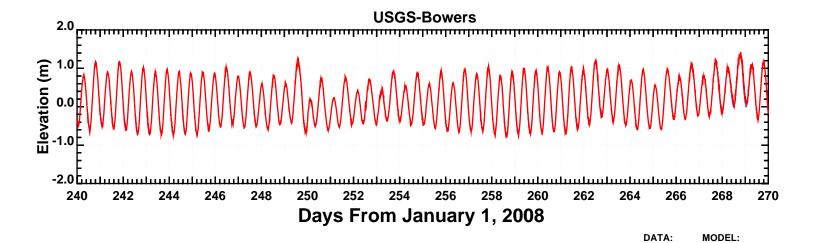
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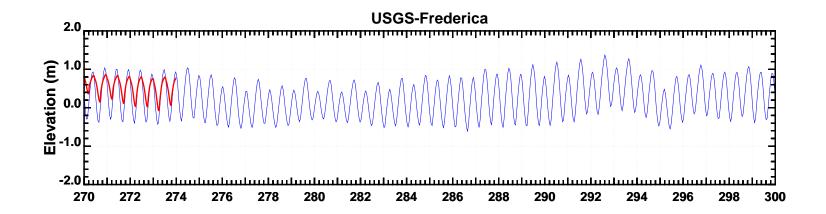


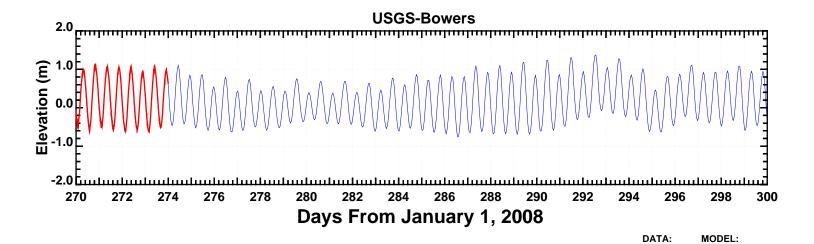
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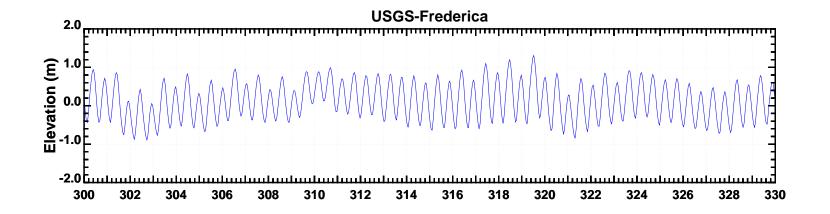


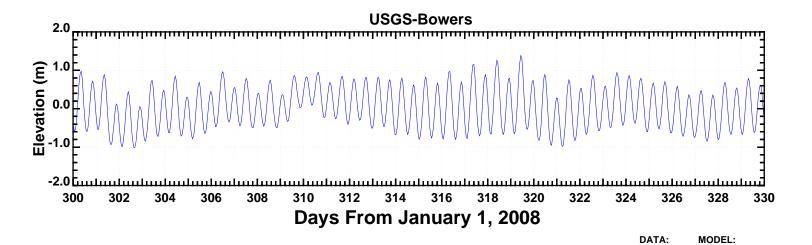
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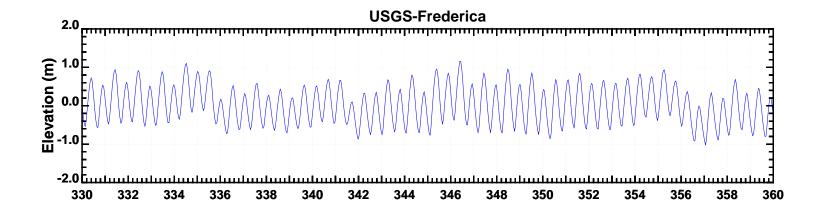


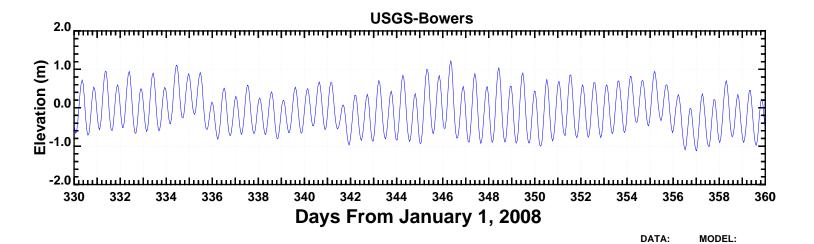
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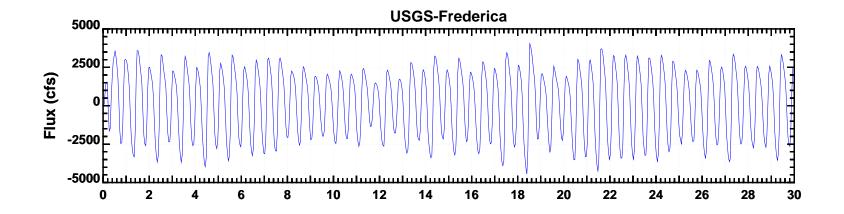


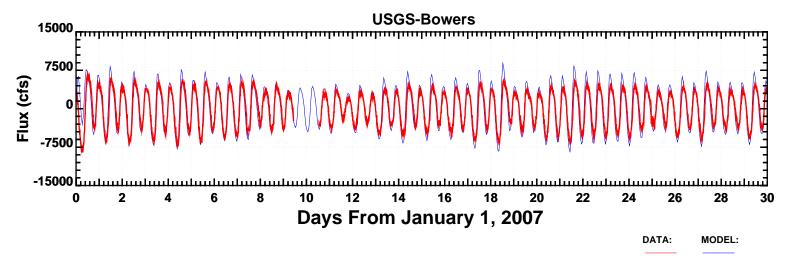


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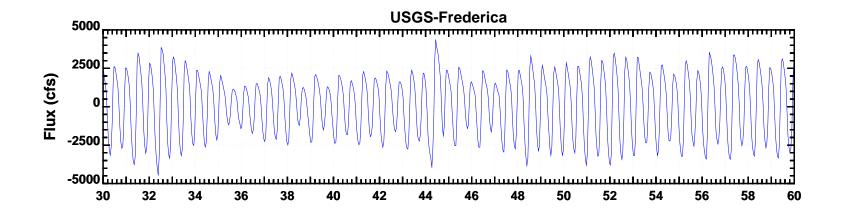
## **APPENDIX 6**

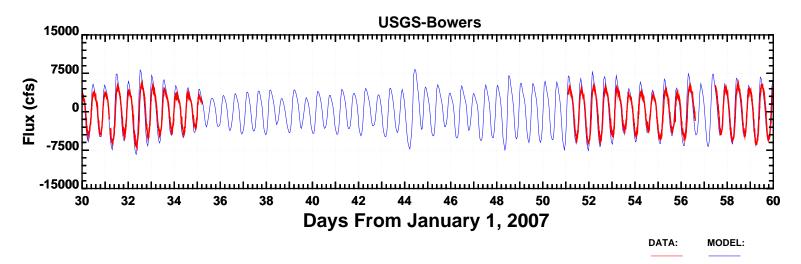
## HYDRODYNAMIC MODEL TIDAL FLUX CALIBRATION/VALIDATION FIGURES



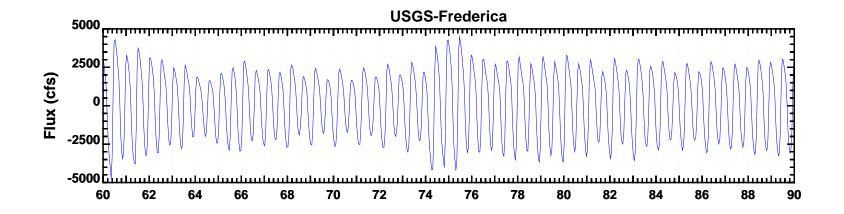


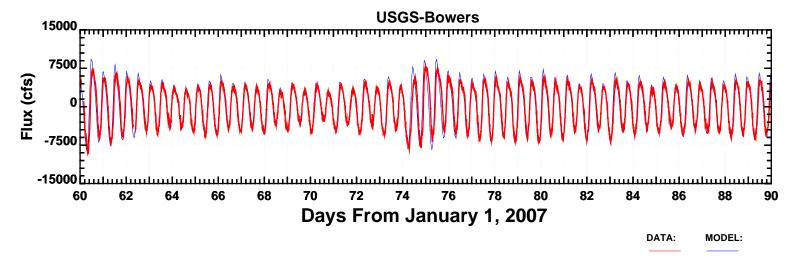
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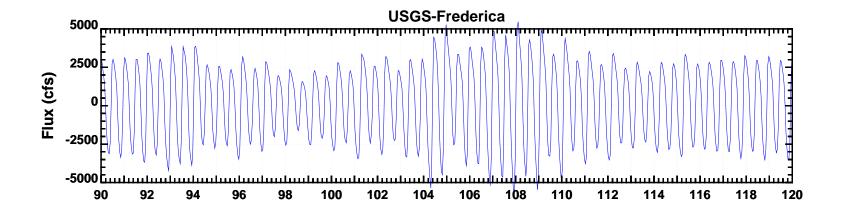


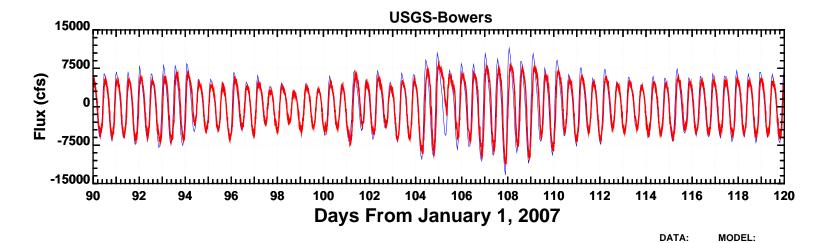
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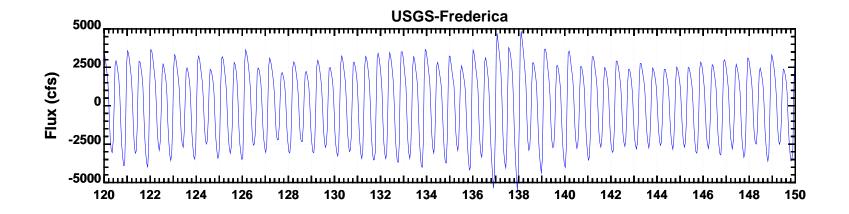


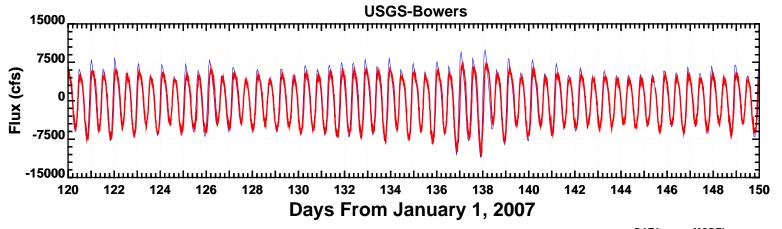
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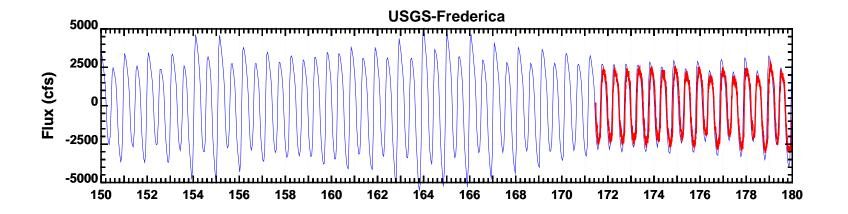
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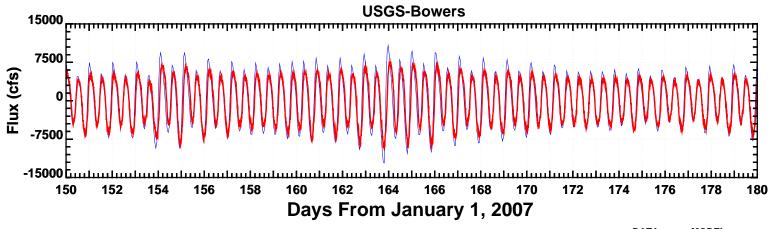




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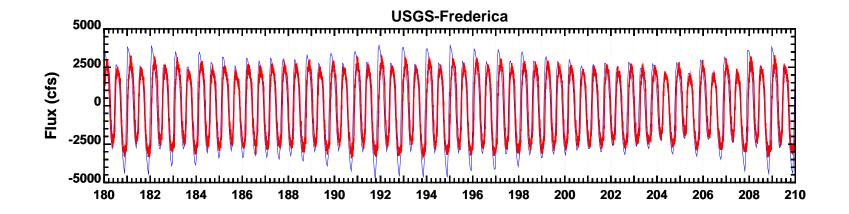
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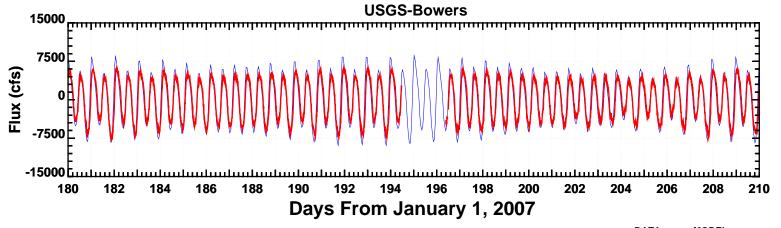




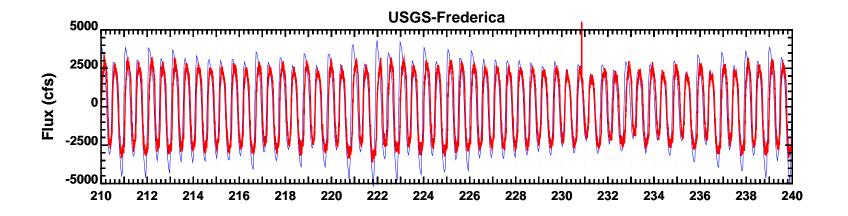
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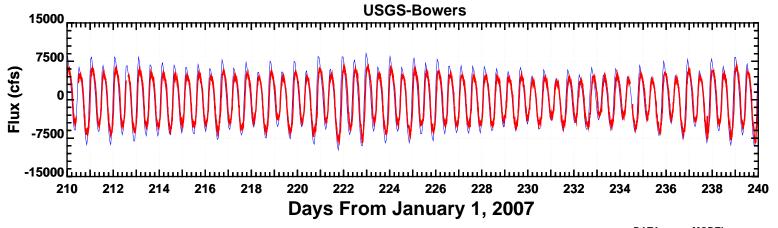
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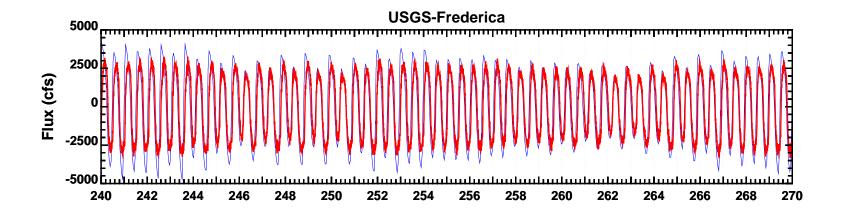


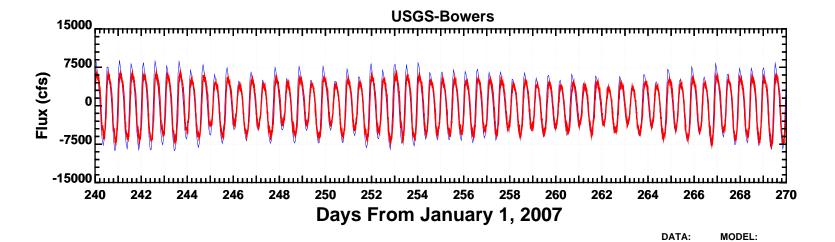
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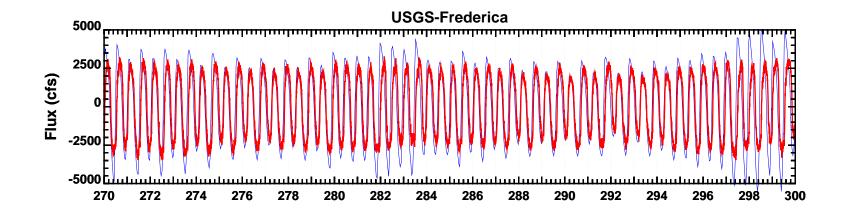


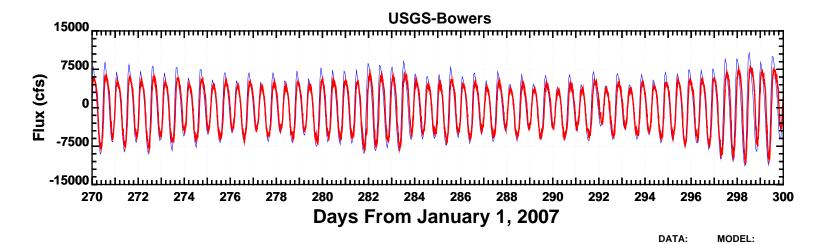
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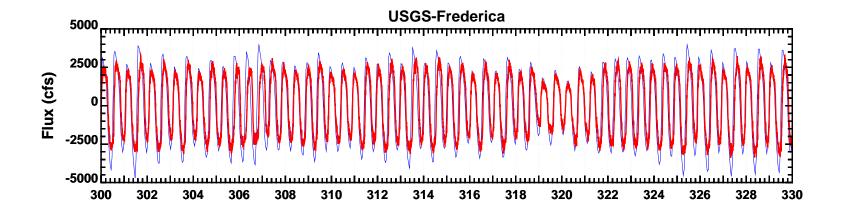


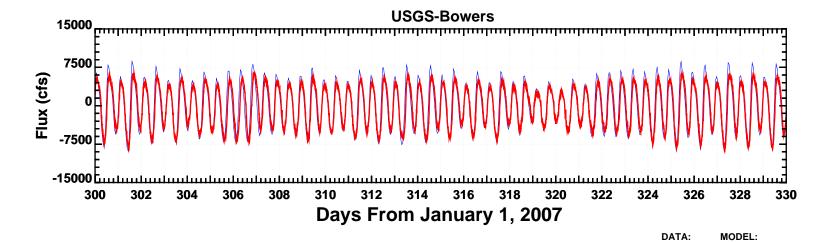
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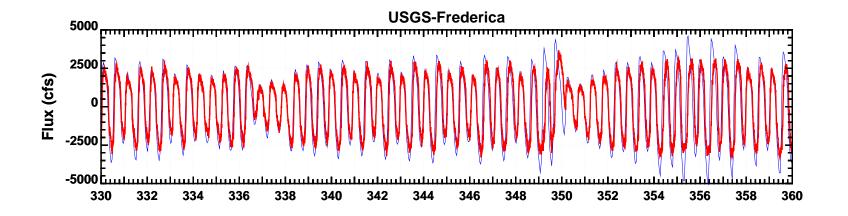


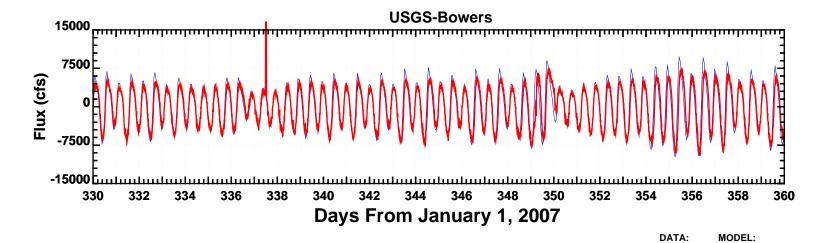
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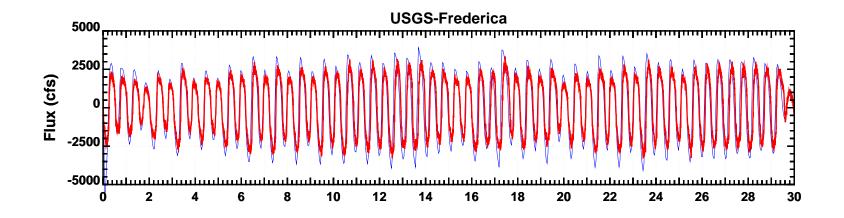


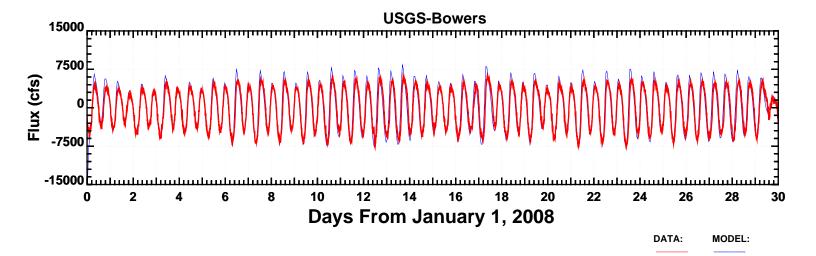
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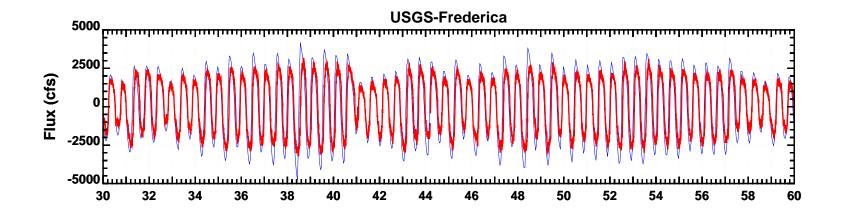
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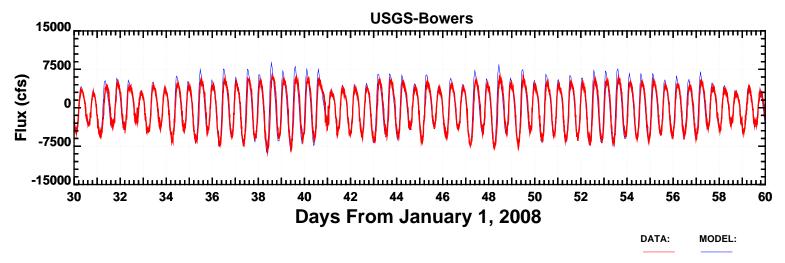




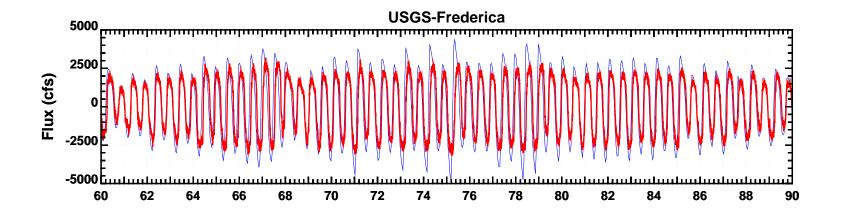
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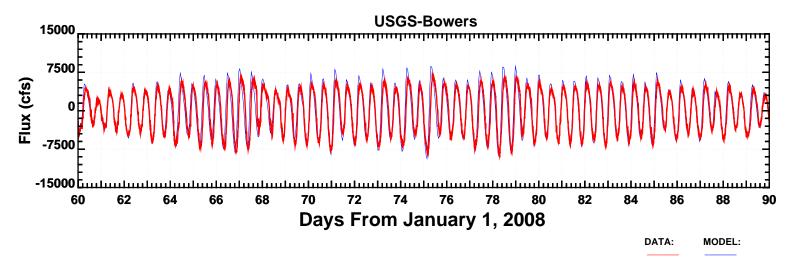
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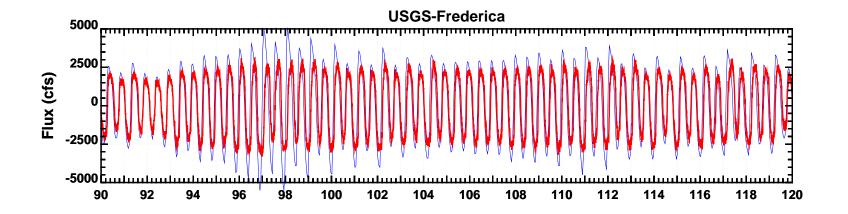


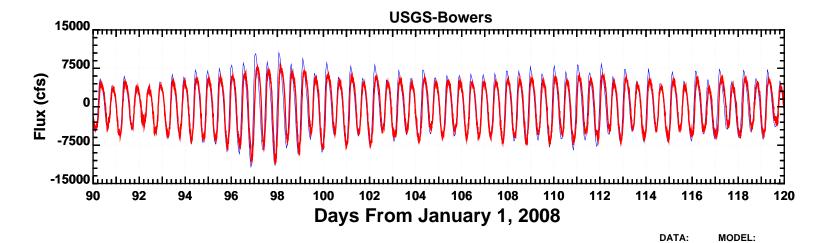
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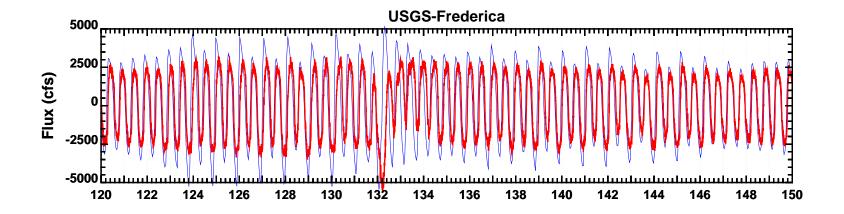


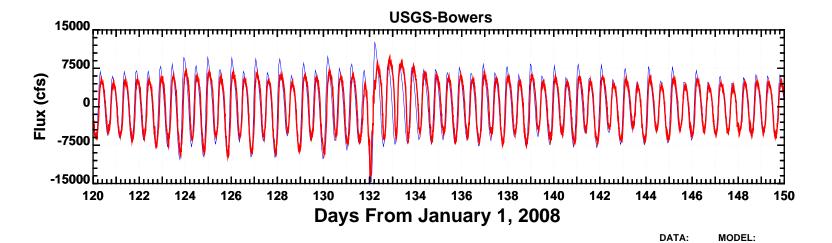
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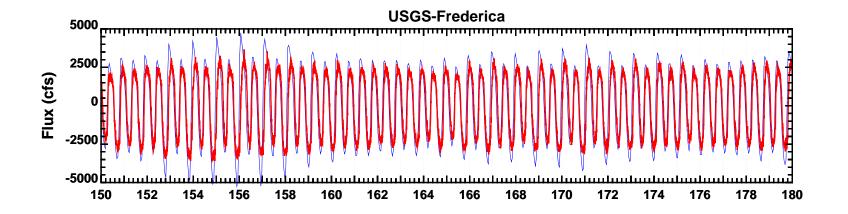
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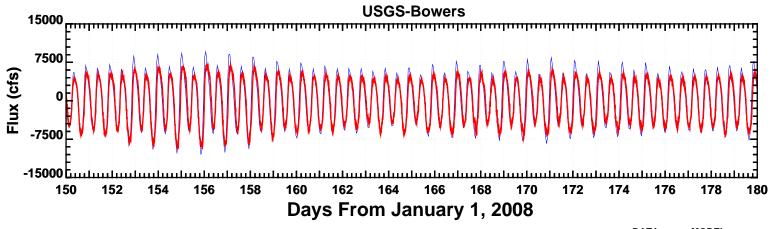




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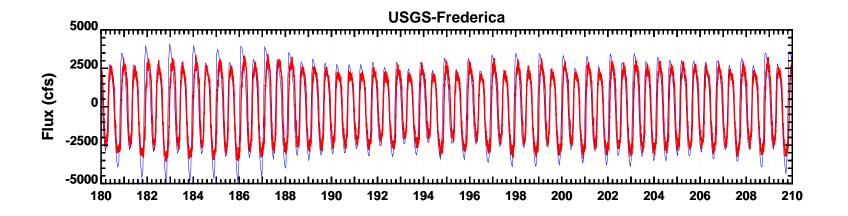
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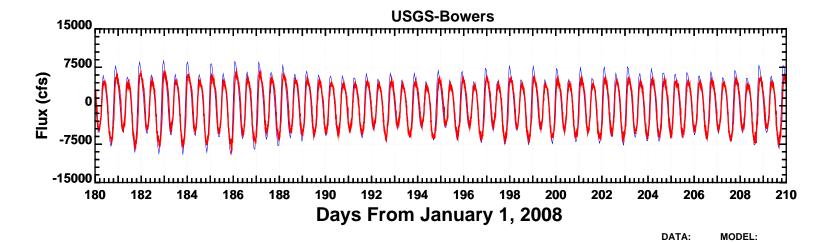




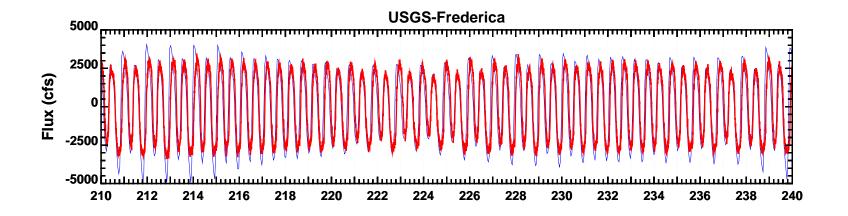
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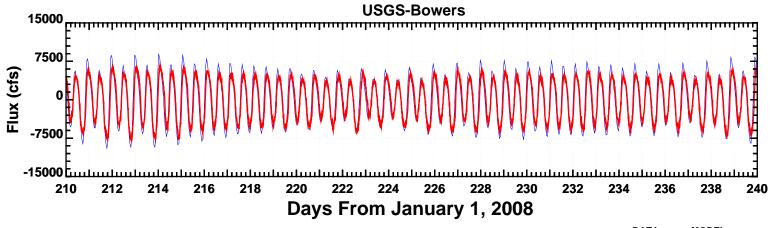
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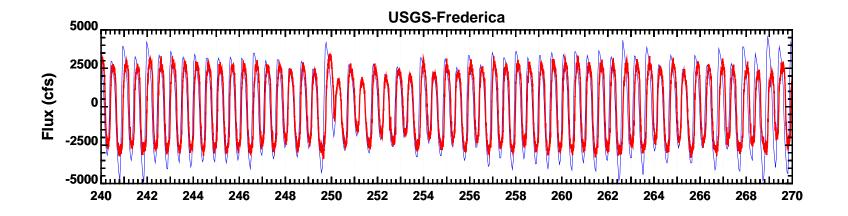


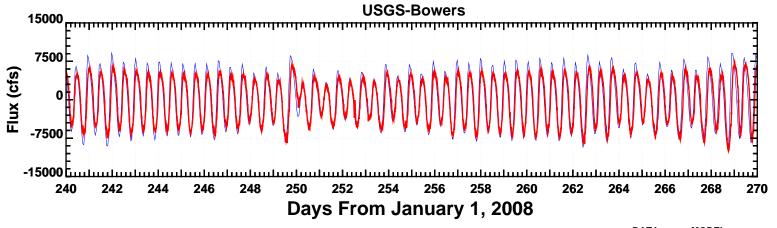
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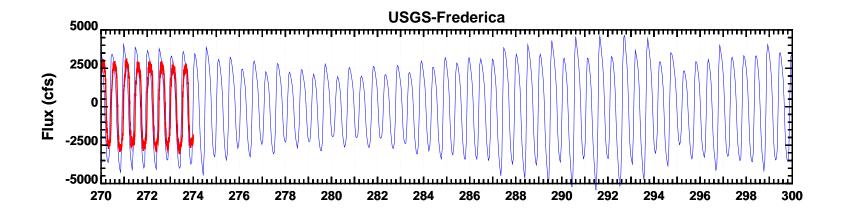


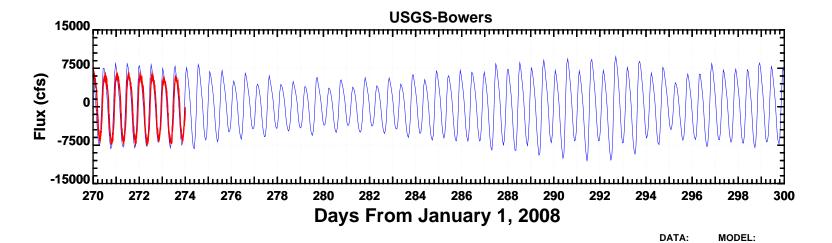


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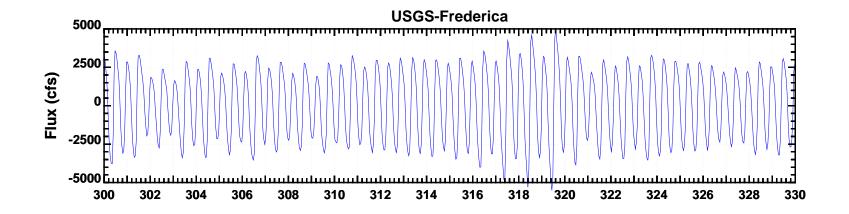
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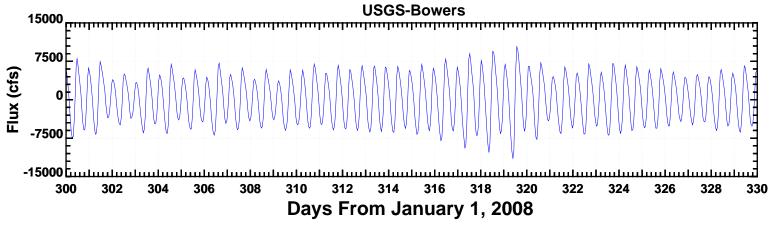




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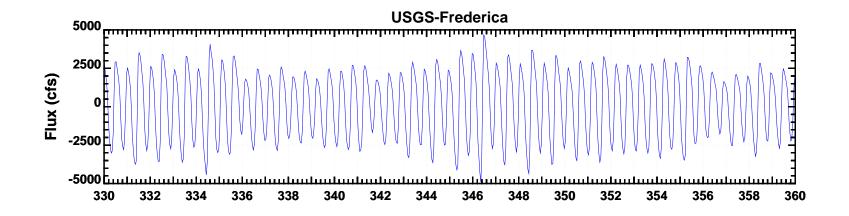


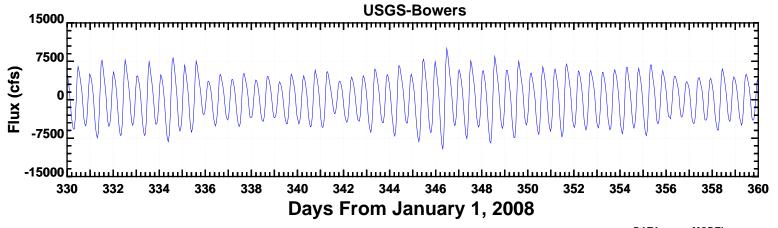


DATA: MODEL:

DNREC Study

/birch1/kcdw0014/HYDRO/PLOTS/FLUXES/fluxReport.gdp





DATA: MODEL:

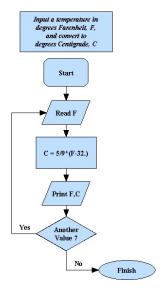
DNREC Study

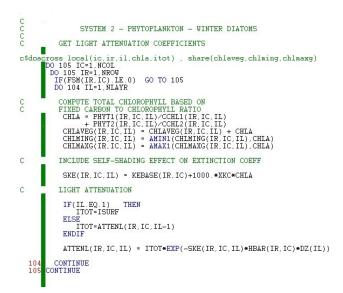
/birch1/kcdw0014/HYDRO/PLOTS/FLUXES/fluxReport.gdp

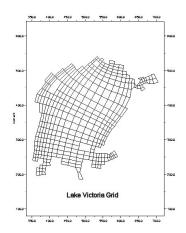
# APPENDIX 7 RCA DOCUMENTATION

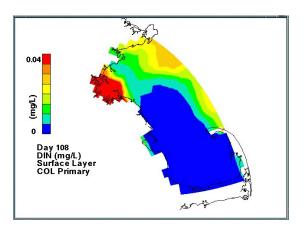
# USER'S GUIDE FOR RCA (Release 3.0)

#### **JUNE 2004**











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VERSION 3.0 OF RCA



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#### **PREFACE**

The purpose of this manual is to describe the inputs (and their associated formats) required to use the generalized HydroQual water quality model, RCA (an acronym for Row-Column AESOP). The manual also documents the procedure to follow to generate an executable version of the RCA program.

RCA is an extension to the family of generalized water quality models developed by HydroQual (and its predecessor firm Hydroscience). The original member of the family was known as WASP (Water Analysis Simulation Program) and was developed in the early 1970s at Hydroscience. This program was later provided to the U.S. EPA and continues to be supported by the EPA's Center for Water Quality Modeling. The most recent version is WASP6. The second generation of the family is known as AESOP (Advanced Ecological Systems Modeling Program) and was also developed by Hydroscience in the mid- to late-1970s. AESOP provided considerable improvements over the original WASP code including: a more computationally efficient numerical integration scheme (implicit integration); a more flexible computer coding approach for generating variable-configuration versions (i.e., number of systems by number of segments) of the code; addition of system dependent transport; and, in the mid-1980s, a preliminary link to HydroQual's generalized circulation model, ECOM, which was developed by Blumberg and Mellor (1987).

The newest member of the family, RCA (Row-Column AESOP), is meant to provide a WASP/AESOP-compatible computational framework for fine-mesh grids that can be used in conjunction with hydrodynamic applications for large lakes, rivers, and estuarine and coastal systems. RCA is able to directly interface with ECOM and ECOMSED and utilizes the same model grid and geometry and bathymetric information as used by the hydrodynamic model. RCA uses the transport fields that result from the hydrodynamic computation to compute the transport of water quality variables of interest within the study domain. In addition, since computing water quality on the same grid as used by the hydrodynamic model can be computationally expensive, options exist within RCA to take advantage of grid-aggregation programs. These grid-aggregation programs provide the user with a means of aggregating or collapsing the fine-grid hydrodynamic model into a coarser-grid representation suitable for water quality computational purposes.

Since RCA is a descendant of AESOP, much of the input structure and nomenclature is the same as is incorporated in AESOP. Therefore, a user familiar with AESOP should be able to set up a RCA input file without too much difficulty.



The interfacing between RCA and ECOM has been checked extensively (and recognition is extended to Kai-Yuan Yang and Eugenio Gomez-Reyes for their concerted efforts in this task) in this release of RCA. RCA has been demonstrated to exactly reproduce salinity fields computed by the ECOM/ECOMSED model, when run using the same integration procedure (the center-differenced in time and space, leap-frog scheme) as ECOM/ECOMSED. RCA also compares favorably to ECOM/ECOMSED salt computations when run using the upwind or backward difference scheme with Smolarkiewicz correction applied.

As stated above the purpose of this manual is to document the model inputs and input structure required to set up and perform a water quality simulation using RCA. As such the user's guide provides a brief description of the required input fields, the associated units (e.g. m/sec, kg/day, etc.) expected by RCA, and the input options available to the user should more than one type of input for a input group be permitted.

All ideas and critical comments concerning improvements (typos, sections requiring greater clarity in writing and purpose, etc.) which could be made to this document are welcomed by its author and should be directed to the undersigned. Kai-Yuan Yang is also recognized for his valuable contributions in integrating the various "versions" of RCA that have been spawned since RCA Version 2.0 into the new RCA 3.0 documented in this manual. Linda Jensen is also recognized for her patience and perseverance in preparing this Users Guide.

James J. Fitzpatrick



#### 1.0 Introduction

RCA is a Row-Column version of AESOP, HydroQual's general purpose water quality modeling computer code. RCA was developed to directly interface with HydroQual's general circulation model, ECOMSED. As such, it will eliminate the need to use ECOSOP, the hydrodynamic to water quality model interface program that is required to link ECOMSED and AESOP.

Both RCA and AESOP solve general mass balance equations for water quality variables of interest. The principle difference between RCA and AESOP is that RCA obtains it advective and dispersive transport fields from a hydrodynamic model, whereas in AESOP the transport fields are specified by the user, based on kinematic box analysis or via calibration to a conservative tracer variable such as salinity.

A second difference between the two computer codes is that RCA has been written to take advantage of the parallel processing capabilities of CRAY or SGI computer systems and, therefore, should be faster than an equivalent AESOP model with the same number of segments.

#### 1.1 Characteristics of the Model

#### Generality

RCA (as is AESOP) is a general purpose code developed to be used to evaluate a myriad of water quality problem settings. The user is able, via the development of a FORTRAN subroutine, to tailor RCA to address the specific water quality issues of the water body under investigation. The FORTRAN subroutine (called TUNER) prescribes the biological, chemical and/or physical kinetics or interrelationships between the relevant water quality variables of interest.

#### Mass Balance

RCA formulates mass balance equations for each model segment for each water quality constituent or state-variable of interest. These mass balance equations include all horizontal, lateral and vertical components of advective flow and dispersive mixing between model segments; physical, chemical and biological transformations between the water quality variables within a model segment; and point, nonpoint, fall-line and atmospheric inputs of the various water quality variables of interest.

#### Finite Difference

The partial differential equations, which form the water quality model, together with their boundary conditions, are solved using mass conserving finite difference techniques, Equation 1.



$$\frac{dM_{i}}{dt} = C_{i} \frac{dV_{i}}{dt} + V_{i} \frac{dC_{i}}{dt}$$
(1a)

$$\frac{dV_{i}}{dt} = \sum Q_{in} - \sum Q_{out}$$
 (1b)

$$\begin{split} \frac{dC_{i}}{dt} &= \sum \frac{Q_{in}}{V_{i}} \left( \alpha \ C_{up} + (1 - \alpha) \ C_{i} \right) - \sum \frac{Q_{out}}{V_{i}} \left( \alpha \ C_{i} + (1 - \alpha) \ C_{dwn} \right) \\ &+ \sum \frac{R_{ij}}{V_{i}} \left( C_{j} - C_{i} \right) + \frac{W_{i}}{V_{i}} \pm k_{i} \ C_{i} \end{split} \tag{1c}$$

where

 $M_i$  = mass of substance in segment i (kg),

 $C_i$  = concentration of substance in segment i (mg/L),

 $V_i$  = volume of segment i (m<sup>3</sup>),

t = time,

 $Q_{in}$  = flow(s) entering segment i (m<sup>3</sup>/sec),

Q<sub>out</sub> = flow(s) leaving segment i (m<sup>3</sup>/sec),

 $\alpha$  = weighting or differencing factor,

= 1 for upwind scheme,

= 0.5 for central differencing scheme,

 $C_{up}$  = concentration of substance entering segment i due to  $Q_{in}$ , i.e., the

concentration in the "upstream" segment (mg/L),

C<sub>dwn</sub> = concentration of substance in the "downstream" segments

associated with Q<sub>out</sub> (mg/L),

 $R_{ii}$  = bulk exchange coefficient between segments i and j (m<sup>3</sup>/sec),

C<sub>j</sub> = concentration of substance in segment j (mg/L),

 $W_i$  = load or source input of substance i (kg/day),

 $k_i$  = reaction of substance in segment i (day<sup>-1</sup>).

Each water quality segment or grid cell is assumed to be completely mixed, i.e., the concentrations of each water quality variable are uniform within the model segment or grid cell. Two finite difference approximations are available for the space derivatives: central difference, which introduces little or no artificial diffusion; and backward or upwind difference, which introduces an artificial diffusion that is proportional to the advective velocity and the grid size, as per Equation 2:

$$E_{num} = \frac{u\Delta x}{2} \tag{2}$$

where

E<sub>num</sub> is the artificial or numerical diffusion (m<sup>2</sup>/sec), u is the advective velocity (m/sec),



 $\Delta x$  is the grid spacing (m).

Ideally, one would want to utilize central difference approximations in water quality modes, since no artificial diffusion is introduced into the model solution. However, the use of central differences can introduce other "problems" (but not errors) into the solution of the model equations. In particular, the use of central differences does not guarantee positivity, i.e. "negative" concentrations can be computed, although mass is conserved. Nor do central differences resolve step functions or delta functions, as might be introduced by point source inputs or intermittent CSO inputs, in a desirable fashion. The specification of these "abrupt" inputs can result in the generation of "saw-toothed" solutions, i.e. small oscillations about the mean concentration profile, along a spatial gradient, or "in a purely advective system" the apparent propagation of concentration upstream of a pollutant discharge. Again, these characteristics are not "errors" in the solution, but rather undesirable features resulting from the use of central differences in an attempt to eliminate numerical dispersion. While the central difference algorithm is available for use in RCA applications, it is recommended that it not be used because of the aforementioned problems.

As noted above, backward or upwind finite difference approximations to the continuous partial differential mass balance equation are also included as an option in RCA. While upwind differences do maintain positivity and do not generate "saw-toothed" solutions, they do introduce numerical dispersion into the finite difference equations. For certain problems, the magnitude of this numerical dispersion might be sufficient to eliminate or significantly reduce concentration gradients in the vertical or horizontal planes. To partially alleviate this problem, RCA has been coded with an additional user selectable option that permits the use of an upwind corrector scheme, based on Smolarkiewicz's antidiffusive velocity algorithm, which reduces the magnitude of the numerical dispersion in the finite difference solution. While this option can significantly improve the resolution of vertical and horizontal concentration gradients by RCA, it does so at the cost of additional computational overhead (20 to 50 percent increases in run-time).

#### Solution Options

RCA provides the user with a number of numerical schemes for solving the water quality mass balance equations. In time-variable mode, the user may utilize one of five explicit time-stepping algorithms, all of which require that the time-step  $(\Delta t)$  obey Equation 3:

$$\Delta t \leq Min \left( \frac{V}{\sum Q + \sum R + kV} \right) \tag{3}$$

where

 $\Delta t$  is the maximum time-step or integration interval (secs),

V is the segment volume (m<sup>3</sup>),

 $\sum$ Q is the sum of the advective fluxes leaving the segment (m<sup>3</sup>/sec),



 $\sum$ R is the sum of the dispersive fluxes leaving the segment (m<sup>3</sup>/sec), kV is the loss rate of material due to kinetic reactions (m<sup>3</sup>/sec).

The five algorithms include: (1) a centered-in-time Smolarkiewicz-corrected upwind scheme; (2) forward-in-time (first order Euler) with and (3) without Smolarkiewicz correction upwind schemes; (4) and split-timestep with and (5) without Smolarkiewicz correction upwind schemes.

Two modifications have been implemented within RCA to reduce run times for computationally-intensive applications. First, an option to evaluate the kinetic portion of the mass balance equation on a less frequent basis than the transport portion of the equation is evaluated and, second, a split-timestep integration procedure. The first modification assumes that the kinetics or reaction rates of the problem have much lower time constants than do the transport, i.e., the biological or chemical reaction rates on the order of 0.01 to 0.2/day versus equivalent transport rates of 1 to 10/day or greater (equivalent to detention times of 1 to 0.1 days or less). If, for example, a model investigation of eutrophication requires a timestep of 0.01 day (about a quarter hour) to meet the stability criteria of Equation 3, a user might wish to select the option in RCA which permits the kinetic subroutine (TUNER) to be evaluated every 0.10 days, rather the 0.01 day required for the transport. Selecting this option might permit a savings of 20 to 30 percent of the runtime. However, it is recommended that all final calibration runs and all projection runs be performed with the kinetic routine called every transport timestep. This ensures that no "errors" are introduced into the model solution. One way to determine the maximum stepsize for evaluating the kinetic subroutine is to perform a number of simulations, wherein the stepsize for evaluating the kinetics is increased each time and the computational results are compared against a run wherein the kinetic and transport stepsizes are the same, i.e., the base case. The user could then pick a stepsize value for evaluating the kinetics, which minimizes computer runtime, but does not significantly affect the computational results relative to the base case.

The second modification (available in the "in-house" version of RCA), split time-step integration, permits the integration of the "critical detention time" segments using a small timestep to maintain stability for the critical segments, while integrating the remaining (majority) of the water quality segments using a larger (factor of 5 to 10) timestep than is required for the critical segments. One of the options available in RCA is to have RCA step through the entire simulation period (or hydrodynamic transport file) to determine the critical integration timesteps for each averaging period within the hydrodynamic record. This diagnostic analysis provides the absolute "critical" timestep required to maintain stability (as defined by Equation 3) and, in addition the critical timestep for 1, 5, 10, 15 and 20 percent of the computational water quality grid. For example, a water quality grid with 5,000 segments might have the following "average" critical timestep characteristics: an absolute critical timestep of 0.0057 days; 1 percent (50 segments) with a critical timestep of 0.012 days or less; 10 percent (500 segments) with a critical timestep of 0.021 days or



less; 15 percent (750 segments) with a critical timestep of 0.026 days or less; and 20 percent (1000 segments) with a critical timestep of 0.031 days or less. The user could, then, using the appropriate RCA input options, select a critical or split timestep of 0.005 days and a full timestep of 0.025 days (and possibly further select a kinetic subroutine timestep of 0.10 days). This could result in an overall 50 to 75 percent reduction in total computational time over the base case, where all segments are integrated using a timestep of 0.005 days and a kinetic timestep of 0.005 days. Once again the user is urged to perform a number of runs in order to evaluate the sensitivity of the model solution to the split time-step integration stepsize.

#### Variable Grid Size and Sigma-Level and Z-Level Coordinates

Since RCA depends upon the hydrodynamic model, ECOMSED, for its model geometry and transport fields, it employs the same variable horizontal grid and vertical (either sigma- or Z-level) coordinate system as does ECOMSED. (For further information on sigma coordinates and the HydroQual general circulation model the user is referred to the ECOMSED Primer.) While the user may run RCA using a sigma-level coordinate system, RCA will still permit the user to specify boundary condition and initial condition inputs using standard (or fixed depth) levels. RCA then transforms the standard level inputs to the sigma-level grid using linear interpolation.

#### Flexible Specification of Pollutant Inputs

RCA permits the user to specify pollutant inputs using any or all of four categories: point source (WWTPs/CSOs/SSOs), nonpoint source (urban/agricultural/watershed runoff), fall-line or riverine sources, and atmospheric source (wetfall/dryfall). Although all pollutant inputs could be organized and input into the model as one loading group, as is done in AESOP, it was thought that permitting these four groupings in RCA would provide the user with greater flexibility in structuring his/her input deck. By splitting the inputs into four groups, the user can perform sensitivity or component analysis much easier by just setting the scale factor for the appropriate group to the desired value rather than be forced to edit the input file and modify a large group of numbers that correspond to the loading group to be analyzed. An example of this would be to reduce all STP and CSO inputs by fifty percent but keep all non-point source, riverine and atmospheric loadings the same. To do this the user would need only to set the scale factor of the point source loading group to 0.5, leaving all other inputs to the model the same.

#### Flexible Disk Storage of Computational Results

RCA permits the user two types of storage for computational results: (1) domain-wide or "global" dumps of all state-variables at "coarse" time intervals; and/or (2) detailed dumps for selected segments at "fine" time intervals. In the first instance a user could save concentrations for all state-variables over the entire model domain for a period of a year using 10 day intervals. This would permit the user using the HydroQual post-processing tool H4D to generate contour plots or time-variable movies for any plane within the model. When using detailed dumps a user



can generate more detailed information concerning model performance by saving secondary variables, such as total extinction coefficients, nutrient limitation terms, etc., as well as the state-variable concentrations for selected segments within the model, at one day intervals. The user could then generate detailed time-series plots using HydroQual post-processing tool GDP. (Note: the information contained in the detailed dumps is determined in the TUNER subroutine via a series of CALLs to the subroute RCAWBUF. A more complete description of the structure of the RCA output files is contained in Appendix D.)

#### Enhancements to RCA Version 3.0

A number of enhancements have been made between this release of RCA (Version 3.0) and previous versions of the code. These include:

- implementation of an integer "clock" to control the overall numerical simulation and the updating of hydrodynamic, load, and boundary condition inputs,
- a revised input structure for specifying point, nonpoint, and fall line loads that includes provision for specifying a load identification table,
- implementation of piece-wise linear interpolation of load inputs,
- greater checking for input errors, and
- use of comment or header records for input records to facilitate editing or modification of required input information.

In previous versions of RCA a real-time clock (in days) was used by RCA to keep track of the simulation time and coordinate with updating of time-variable models inputs such as generated by the hydrodynamic model ECOMSED or loadings and/or boundary conditions. Unfortunately, the use of REAL variables can result in numerical round-off errors after repeated addition of fractions. This can result in synchronization errors when updating the hydrodynamic model inputs. Therefore, RCA has been modified to use INTEGER variables to specify the numerical time-step for integration and to keep track of the simulation time. These internal variables will operate in units of seconds.

RCA has also been modified so that pollutant loads can be specified using piecewise linear interpolation rather than just step function changes. As an example suppose a user specifies the following time-series input for a pollutant load:

<u>value</u>	<u>time</u>	<u>value</u>	<u>time</u>	<u>value</u>	<u>time</u>
10.0	0.0	20.0	50.0	40.0	100.

If the user selected the step-function option, the value of the pollutant load at time = 25 would be 10.0. If, however, the user selected piece-wise linear interpolation the value at time = 25 would be 15.



Version 3.0 of RCA has also been improved to provide greater checking of model inputs. For example, RCA will check to make sure that the model segment to which a pollutant load is assigned is a valid water cell.

Finally, for normal Ascii (or card-image) files, RCA has been modified to include a "comment" or "header" record to be read before every major input record. Although the user may leave these records "blank" without any consequence, use of these comment records to list or describe the input data to follow may facilitate subsequent editing or modification of the input data required to run the model. It should be noted, however, that comment or header records SHOULD NOT be included in binary files.

#### 1.2 Getting Started

#### Hydrodynamic Model Files

In order to begin, the user will, of course, need a hydrodynamic model. The hydrodynamic model code, ECOMSED, generates three output files (four, if the user chooses to save only the water cells of the model grid) which are required by RCA. These files are named, "gcm\_geom," which contains information concerning model geometry, "gcm\_tran" which contains the advective and dispersive transport fields, and "gcm\_gdiff' which contains information relating to the locations and time-variable discharge volumes associated with any diffusers or outfalls included in the hydrodynamic model (and "wet\_grid," which contains the locations of the water cells in the model domain, if the "water cells only" option is chosen). The user will need to move, copy, or link the "gcm\_geom" and "wet\_grid", if appropriate, files to the directory in which the water quality model and the executable version of RCA are to reside. The "gcm\_tran" file(s) and "gcm\_gdiff" file(s), however, need not be moved, copied, or linked. They can remain in a separate directory, file folder, or disk drive.

#### **TUNER Subroutine**

Next the user will be required to supply a FORTRAN subroutine, which contains the state-equations or kinetics for the water quality problem of interest. The subroutine should be called "TUNER" (as in SUBROUTINE TUNER) but may be maintained on the system using any name that the user desires (for example, lisem2.f). An example TUNER, written for a one-system conservative tracer, which can also be used to calculate residence time of a waterbody (and which can be easily expanded to three-systems) is presented in Table 1. Appendices A and B provide descriptions of more complex TUNERS; one that is HydroQual's current implementation of eutrophication kinetics and one that is HydroQual's current implementation of coliform kinetics and that are provided as part of the public domain release of RCA. Appendix C provides more detail on the residence time subroutine presented in Table 1.



TA	BLE 1	. EXAMPLE	ELISTING OF A KINETIC SUBROUTINE - TUNER	
	*****	*****	***********	**
С	SU	JBROUTINE	TUNER	
	*****	*****	**********	**
C			CE TIME MODEL - COMPUTE RESIDENCE TIME OF A SEGMENT(	s)
0000			ote: current version is set up for 1 system, but may be readily expanded to 2 or 3 systems by uncommenti the appropriate FORTRAN statements in the code)	
	*****	*****	***********	**
C	SY	STEMS	UNI	
C C		1 - DYE1 2 - DYE2 3 - DYE3	- CONCENTRATION OF DYE MG - CONCENTRATION OF DYE MG	G/L G/L G/L
	****	*****	************	**
000	CC	NSTANTS		
С	NO	NAME	DESCRIPTION UNI	TS
000000000	1	DYEDIS1	DYE DISTRIBUTION OPTION  = 0, ASSIGN INITIAL DYE CONCENTRATIONS UNIFORMLY THROUGHOUT THE WATER COLUMN (I.E., TOP TO BOTTOM) USING PARAM2D(1) PARAM2D(2) WILL BE USED TO SPECIFY THE DOMAIN OVER WHICH THE RESIDENCE TIME WILL BE COMPUTED  = 1, INITIAL DYE CONCENTRATIONS WILL BE SPECIFIED ON A SEGMENT BY SEGMENT BASIS USING PARAM3D(1) PARAM3D(2) WILL BE USED TO SPECIFY THE DOMAIN	
C C	2	TIMEDYE1	OVER WHICH THE RESIDENCE TIME WILL BE COMPUTED TIME TO RELEASE DYE 1	,
0 0 0	3 4	DECAY1 DYEDIS2	DECAY RATE FOR DYE 1  DYE DISTRIBUTION OPTION  = 0, ASSIGN INITIAL DYE CONCENTRATIONS UNIFORMLY THROUGHOUT THE WATER COLUMN (I.E., TOP TO	ΑY
000000			BOTTOM) USING PARAM2D(3) PARAM2D(4) WILL BE USED TO SPECIFY THE DOMAIN OVER WHICH THE RESIDENCE TIME WILL BE COMPUTED 1, INITIAL DYE CONCENTRATIONS WILL BE SPECIFIED ON A SEGMENT BY SEGMENT BASIS USING PARAM3D(3) PARAM3D(4) WILL BE USED TO SPECIFY THE DOMAIN OVER WHICH THE RESIDENCE TIME WILL BE COMPUTED	
C	5 6	TIMEDYE2 DECAY2	TIME TO RELEASE DYE 2 DECAY RATE FOR DYE 2 /D	ΑY
000000000	7	DYEDIS3	DYE DISTRIBUTION OPTION  = 0, ASSIGN INITIAL DYE CONCENTRATIONS UNIFORMLY THROUGHOUT THE WATER COLUMN (I.E., TOP TO BOTTOM) USING PARAM2D(5) PARAM2D(6) WILL BE USED TO SPECIFY THE DOMAIN OVER WHICH THE RESIDENCE TIME WILL BE COMPUTED  = 1, INITIAL DYE CONCENTRATIONS WILL BE SPECIFIED ON A SEGMENT BY SEGMENT BASIS USING PARAM3D(5) PARAM3D(6) WILL BE USED TO SPECIFY THE DOMAIN	
C	8	TIMEDYE3	OVER WHICH THE RESIDENCE TIME WILL BE COMPUTED TIME TO RELEASE DYE 3	)
C	9	DECAY3		AY
C* C C		-********** -D PARAMETE	**************************************	**
C		NO NAME	DESCRIPTION UNI	TS
C	_	1 DYE1IC		 
C		2 DOMAIN 3 DYE2IC	2 INITIAL CONDITIONS FOR DYE2 MG	J/L
CCC		4 DOMAIN 5 DYE3IC 6 DOMAIN	2 DOMAIN FOR DETERMINING RESIDENCE TIME 2 2 INITIAL CONDITIONS FOR DYE3 MG	3/L
С	****		3 DOMAIN FOR DETERMINING RESIDENCE TIME 3	**
C				



```
TABLE 1. EXAMPLE LISTING OF A KINETIC SUBROUTINE - TUNER (Cont.)
         3-D PARAMETERS
MG/L
                                                                                                      MG/L
         TIME-VARIABLE FUNCTIONS
                  NONE
INCLUDE 'RCACM'
         CHARACTER
                          GDNAMES (NOSYS) *8, DDNAMES (5, NOSYS) *8
C
              STATE-VARIABLES
         REAL
                  DYE1 (NX, NY, NZ)
               , DYE2(NX,NY,NZ)
CC
                  DYE3 (NX, NY, NZ)
        EQUIVALENCE
(CARAY(1,1,1,1),DYE1(1,1,1))
(CARAY(1,1,1,2),DYE2(1,1,1))
(CARAY(1,1,1,3),DYE3(1,1,1))
CC
CC
         REAL
                  DYE_DDA(NX,NY,NZ,NOSYS)
               , DYE_DMIN(NX,NY,NZ,NOSYS)
, DYE_DMAX(NX,NY,NZ,NOSYS)
               , DYE_GDA(NX,NY,NZ,NOSYS)
         . , DYE1_GDA(NX,NY,NZ)
. , DYE2_GDA(NX,NY,NZ)
. , DYE3_GDA(NX,NY,NZ)
EQUIVALENCE
С
               (DYE_GDA(1,1,1,1),DYE1_GDA(1,1,1))
, (DYE_GDA(1,1,1,2),DYE2_GDA(1,1,1))
, (DYE_GDA(1,1,1,3),DYE3_GDA(1,1,1))
C
C
С
             CONSTANTS
         EQUIVALENCE
              (CONST(1), DYEDIS1) , (CONST(2), TIMEDYE1) , (CONST(3), DECAY1) , (CONST(4), DYEDIS2) , (CONST(5), TIMEDYE2) , (CONST(6), DECAY2) , (CONST(7), DYEDIS3) , (CONST(8), TIMEDYE3) , (CONST(9), DECAY3)
         REAL*8 TOTMASIC (NOSYS), TOTMASREG (NOSYS), TOTMASALL (NOSYS)
         INTEGER*2 SYSGDP(40)
INITIAL -SYSBY- SETTINGS
С
         DATA SYSGDP/40*1/
С
              PROVIDE INITIALIZATION, IF FIRST TIME THROUGH -FABLE-
         PROVIDE INITIALIZATION, IF FIRST TIME THROUGH
IF (INITB.EQ.1) GO TO 50
SET-UP AND WRITE INFORMATION NEEDED BY GDP
GDNAMES (1) = 'DYE1'
GDNAMES (2) = 'DYE2'
С
         GDNAMES(3) = 'DYE3'
DO ISYS=1, NOSYS
             SYSGDP(ISYS) = SYSBY(ISYS)
         ENDDO
         REWIND(10)
         WRITE(10)
                          NX, NY, NZ, NOSYS, NOSYS
GDNAMES
         WRITE(10)
                         SYSGDP
FSM
         WRITE(10)
         WRITE (10)
             WRITE DDNAMES TO RCAF12
         WRITE DDNAMES TO RCAF12
(NOTE: IF SYSTEM 2 AND/OR 3 ACTIVATED ADD APPROPRIATE DDNAMES)
IF(IDDOPT.EQ.0) THEN
DDNAMES(1,1)=' DVE1'
DDNAMES(1,2)=' DUMMY'
DDNAMES(1,3)='IC MASS1'
DDNAMES(1,4)='REGNMAS1'
DDNAMES(1,5)='DOMNMAS1'
FISE
```



#### TABLE 1. EXAMPLE LISTING OF A KINETIC SUBROUTINE - TUNER (Cont.)

```
DDNAMES(1,1)='AVE DYE1'
DDNAMES(1,2)='MAX DYE1'
          DDNAMES(1,3) = 'IC MASS1'
DDNAMES(1,4) = 'REGNMAS1'
DDNAMES(1,5) = 'DOMNMAS1'
         WRITE(12) DDNAMES
        SET INITIAL CONDITIONS
DO 30 ISYS=1,NOSYS
IF(CONST(3*(ISYS-1)+1).EQ.0 .AND. CONST(3*(ISYS-1)+2).EQ.0.) THEN
С
             F(CONSI(3*(ISYS-1)+1).EQ.0 .AND. CONSI(3*(ISYS-1)+2).EQ.0.)
DO 10 IZ=1,NZ
DO 10 IY=1,NY
DO 10 IX=1,NX
IF(FSM(IX,IY).EQ.1.)
CARAY(IX,IY,IZ,ISYS) = PARAM2D(IX,IY,2*(ISYS-1)+1)
    10
             CONTINUE
             CONSTINCE
RESET CONSTANT SO DYE IS NOT PUT INTO SYSTEM AGAIN
CONST(3*(ISYS-1)+2)=9.99E+9
С
          ELSEIF (CONST (3* (ISYS-1)+1).EQ.1 .AND. CONST (3* (ISYS-1)+2).EQ.0.)
           THEN
            DO 20 IZ=1, NZ

DO 20 IY=1, NY

DO 20 IX=1, NX

IF (FSM (IX, IY) .EQ.1.)
                          CARAY(IX, IY, IZ, ISYS) = PARAM3D(IX, IY, IZ, 2*(ISYS-1)+1)
             CONTINUE
    20
          CONST(3*(ISYS-1)+2)=9.99E+9
ENDIF
    30 CONTINUE
         CALL RCA09
IREC=IREC-1
C
             INITIALIZE ARRAY FOR GLOBAL DUMP AVERAGING, IF REQUIRED
         IF(IGDOPT.EQ.1) THEN DO 40 ISYS=1,NOSYS
           DO 35 IZ=1,NZ
DO 35 IY=1,NY
DO 35 IX=1,NX
                 DYE_DDA(IX,IY,IZ,ISYS) = 0.

DYE_DDA(IX,IY,IZ,ISYS) = 0.

DYE_DMIN(IX,IY,IZ,ISYS) = 1000.

DYE_DMAX(IX,IY,IZ,ISYS) = -1000.
            CONTINUE
    40
          CONTINUE
          IAVGGDCNTR = 0
          IAVGDDCNTR = 0
IAVGPPCNTR = 0
         ENDIF
        DUMMY=0.0
    50 CONTINUE
             CHECK IF TIME TO LOAD ANOTHER DYE
        DO 100 ISYS=1, NOSYS
          IF (CONST(3*(ISYS-1)+1).EQ.0 .AND. TIME.GT.CONST(3*(ISYS-1)+2))
             WRITE(OUT,1200) ISYS,TIME
FORMAT(//10X,'LOADING TRACER #',I2,' AT TIME',F8.2)
DO 70 IZ=1,NZ
 1200
              DO 70 IY=1,NY
DO 70 IX=1,NX
CARAY(IX,IY,IZ,ISYS) = PARAM2D(IX,IY,2*(ISYS-1)+1)
    70
             CONTINUE
             CONST(3*(ISYS-1)+2)=9.99E+9
CALL RCA09
             IREC=IREC-1
          ELSEIF (CONST (3* (ISYS-1)+1).EQ.1.AND.TIME.GT.CONST (3* (ISYS-1)+2))
            80
             CONTINUE
             CONST(3*(ISYS-1)+2)=9.99E+9
CALL RCA09
             IREC=IREC-1
          ENDIF
   100 CONTINUE
```

LOOP FOR DETAILED DUMP AVERAGING, IF REQUIRED



#### TABLE 1. EXAMPLE LISTING OF A KINETIC SUBROUTINE - TUNER (Cont.) IF(IDDOPT.EQ.1) THEN DO 125 ISYS=1,NOSYS DO 120 IZ=1,NZ DO 120 IY=1,NY DO 120 IX=1,NX DYE\_DDA(IX,IY,IZ,ISYS) = DYE\_DDA(IX,IY,IZ,ISYS) + CARAY(IX,IY,IZ,ISYS) DYE\_DMIN(IX,IY,IZ,ISYS) = AMIN1 (DYE\_DMIN (IX, IY, IZ, ISYS), CARAY (IX, IY, IZ, ISYS)) DYE\_DMAX (IX, IY, IZ, ISYS) = AMAX1 (DYE\_DMAX (IX, IY, IZ, ISYS), CARAY (IX, IY, IZ, ISYS)) CONTINUE 120 125 CONTINUE IAVGDDCNTR = IAVGDDCNTR + 1 ENDIF SYSTEM 1(-3) - DYE1(-3) DO 150 ISYS=1,NOSYS TOTMASIC(ISYS)=0. TOTMASREG(ISYS) = 0. TOTMASALL(ISYS) = 0. DO 135 IZ=1,NZ DO 135 IY=1,NY DO 135 IX=1,NY IF (FSM(IX,IY).NE.1.) GO TO 135 CDARAY(IX, IY, IZ, ISYS) = -CONST(3\*ISYS)\*CARAY(IX, IY, IZ, ISYS) IF (IDISK.NE.0) THEN IF (CONST(3\*(ISYS-1)+1).EQ.0.) THEN IF (PARAMZD(IX, IY, 2\*(ISYS-1)+1).GT.0.) TOTMASIC(ISYS) = TOTMASIC(ISYS) + BVOL(IX, IY, IZ)\*CARAY(IX, IY, IZ, ISYS) IF (PARAMZD(IX, IY, 2\*ISYS).GT.0.) TOTMASREG(ISYS) = TOTMASREG(ISYS) + BVOL(IX, IY, IZ) \*CARAY(IX, IY, IZ, ISYS) IF(PARAM3D(IX,IY,IZ,2\*(ISYS-1)+1).GT.0.) TOTMASIC(ISYS) = TOTMASIC(ISYS) + BVOL(IX,IY,IZ)\*CARAY(IX,IY,IZ,ISYS) IF(PARAM3D(IX,IY,IZ,2\*ISYS).GT.0.) TOTMASREG(ISYS) = TOTMASREG(ISYS) + BVOL(IX, IY, IZ) \*CARAY(IX, IY, IZ, ISYS) TOTMASALL(ISYS) TOTMASALL(ISYS) + BVOL(IX, IY, IZ) \*CARAY(IX, IY, IZ, ISYS) ENDIF 135 CONTINUE IF(IDISK.EQ.2 .OR. IDISK.EQ.3) THEN DO 145 IDMP=1,NDMPS IX = IFDMPS(IDMP,1) IY = IFDMPS(IDMP,2) IY = IFDMPS(IDMM,Z) IZ = IFDMPS(IDMM,3) IF(IDDOPT.EQ.0) THEN CALL RCAWBUF(ISYS,CARAY(IX,IY,IZ,ISYS),dummy ,SNGL(TOTMASIC(ISYS)),SNGL(TOTMASREG(ISYS)) , SNGL (TOTMASALL (ISYS))) ELSE CALL RCAWBUF(ISYS, CARAY(IX, IY, IZ, ISYS)/IAVGDDCNTR , DYE\_DMAX(IX, IY, IZ, ISYS) , SNGL(TOTMASIC(ISYS)), SNGL(TOTMASREG(ISYS)) ,SNGL(TOTMASALL(ISYS))) ENDIF 145 CONTINUE ENDIF 150 CONTINUE C CONVERT TO MASS UNITS c\$doacross local(iz,iy,ix,isys) DO 200 ISYS=1,NOSYS DO 200 IZ=1,NZ DO 200 IY=1,NY DO 200 IX=1,NX CDARAY(IX,IY,IZ,ISYS) = BVOL(IX,IY,IZ)\*CDARAY(IX,IY,IZ,ISYS) IF(IDISK.EQ.2 .OR. IDISK.EQ.3) CLOSE BUFFER AND WRITE TO DISK CALL RCAWRIT

TOTMASIC(ISYS)/1000., TOTMASREG(ISYS)/1000.

,TOTMASALL(ISYS)/1000.

/10X, 'REGIONAL TOTAL MASS =',E13.5,' KG'/
/10X,'DOMAIN TOTAL MASS =',E13.5,' KG'/)

/10X, 'INITIAL CONDITION REGIONAL TOTAL MASS =', E13.5,' KG'

DO ISYS=1, NOSYS

FORMAT (

2500

WRITE (OUT, 2500)



```
TABLE 1. EXAMPLE LISTING OF A KINETIC SUBROUTINE - TUNER (Cont.)
            RE-INITIALIZE ARRAY FOR DETAILED DUMP AVERAGING, IF REQUIRED IF (IDDOPT.EQ.1) THEN
DO 215 ISYS=1,NOSYS
DO 210 IZ=1,NZ
DO 210 IX=1,NY
DO 210 IX=1,NX
DYE_DDA(IX,IY,IZ,ISYS) = 0.
DYE_DMIN(IX,IY,IZ,ISYS) = 1000.
DYE_DMAX(IX,IY,IZ,ISYS) = -1000.
CONTINUE
CONTINUE
    210
    215
              CONTINUE
              IAVGDDCNTR = 0
             ENDIF
           ENDIF
           ENDIF

PERFORM GLOBAL DUMP AVERAGING, IF REQUIRED

IF (IGDOPT.EQ.1) THEN

DO 225 ISYS=1,NOSYS

DO 220 IZ=1,NZ

DO 220 IY=1,NY

DO 220 IX=1,NX

DYE_GDA(IX,IY,IZ,ISYS) = DYE_GDA(IX,IY,IZ,ISYS)

+ CARAY(IX,IY,IZ,ISYS)
C
   220 CONTINUE
225 CONTINUE
           ENDIF
           IAVGGDCNTR = IAVGGDCNTR + 1
           CHECK IF TIME TO DUMP TO DISK IF(IDISK.EQ.0) RETURN GLOBAL DUMPS
С
           GLOBAL DUMPS
IF(IDISK.EQ.1 .OR. IDISK.EQ.3) THEN
IF(IGDOPT.EQ.0) THEN
WRITE(10) TIME
WRITE(11) DYE1
WRITE(11) DYE2
WRITE(11) DYE2
                WRITE(11) DYE3
           WRITE(II,
ELSE
DO 365 ISYS=1,NOSYS
DO 360 IZ=1,NZ
DO 360 IY=1,NY
DO 360 IX=1,NX
DYE_GDA(IX,IY,IZ,ISYS) = DYE_GDA(IX,IY,IZ,ISYS)/
FLOAT(IAVGGDO
                                                                                            FLOAT (IAVGGDCNTR)
    360
    365
                WRITE(10)
                                       TIME - FLOAT (IPRNTGSECS) /86400./2.
                 WRITE(11)
                                      DYE1_GDA
                WRITE (11)
                                      DYE2 GDA
                 WRITE(11)
                                      DYE3_GDA
             ENDIF
             DO 385 ISYS=1, NOSYS
DO 380 IZ=1, NZ
DO 380 IY=1, NY
                    DO 380 IX=1,NX
                DYE_GDA(IX, IY, IZ, ISYS) = 0.
CONTINUE
    380
               CONTINUE
             ENDIF
            IAVGGDCNTR = 0
IAVGPPCNTR = 0
                INITIAL CONDITION FILE
           REWIND 15
WRITE(15) CARAY
           RETURN
   900 WRITE(OUT,9990)
9990 FORMAT(///5X,'INPUT ERROR WHILE READING IGDOPT,IDDOPT'//)
CALL EXIT
  9990
```



#### Generating a RCA Executable using "makerca3"

In order to use RCA, the user should copy the RCA source code and makerca3 script from App\_Server\Install\RCA to his/her working directory. The user would then execute the "makerca3" script from his/her working directory. This script has options for copying the RCA source code to the working directory, editing various files, compiling the RCA code and building an executable version of RCA. After copying the files, the first task is to edit the "RCACM" file to set the appropriate parameters. These are at the top of the RCACM file in the first PARAMETER statement. The following is a list of variables to be set with a brief description of each:

<u>Variable</u>	<u>Definition</u>
nx	number of grid cells in the x-axis of the model
ny	number of grid cells in the y-axis of in the model
nz	number of grid cells or layers in the vertical plane of
	the model
nosys	number of systems or water quality state-variables

The first few lines of RCACM are listed below:

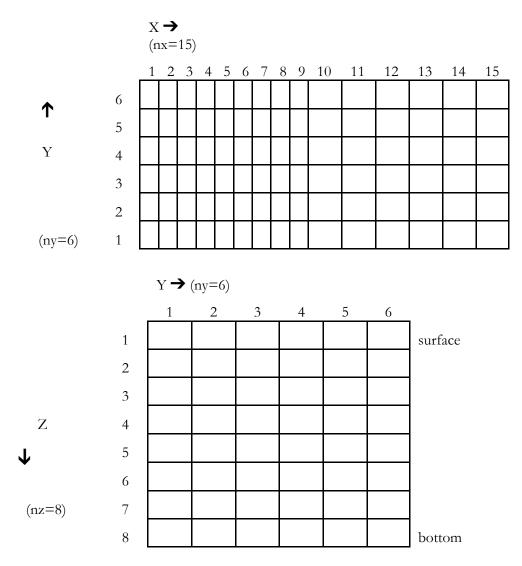
```
C C CONFIGURATION, REAL, INTEGER, AND COMMON CARDS FOR RCA Version 3.0

PARAMETER (NX=nx,NY=ny,NZ=nz,NOSYS=nosys)
PARAMETER (NPARM2D=10,NPARM3D=6,NBC=750,NWK=750)
PARAMETER (MXCONS=250,MXFUNC=20,MXFUNCT=400)
PARAMETER (MXHYDFILES=36,NHYD=15000,NSL=100,NSLC=100)
PARAMETER (MXSEGSPLT=(NX*NY*NZ)/5)
```

The user would then modify "nx, ny, nz" as per the dimensions required for the model being developed.

An example grid is presented below in order to assist the user in understanding the definitions of nx, ny and nz.





The above "hydrodynamic/water quality grid" has 15 cells in the x-direction, 6 cells in the y-direction and 8 vertical layers.

After editing RCACM, the user should copy the appropriate TUNER.f kinetic subroutine to the CODE directory and compile and build an executable version of RCA using either of the following commands:

**df /exe:rca\_ver3 /convert:BIG\_ENDIAN \*.f** for a WINDOWS version of RCA -or- **makerca** for a LINUX (UNIX) version of RCA.



#### 1.3 RCA File Structure

During the course of execution RCA requires a number of input files and generates a number of output files. These are briefly described in Table 2. Further details concerning these files will be provided in the following section.

**TABLE 2. RCA FILE STRUCTURE** 

#### A. USER CREATED INPUT FILES

	NAME	TYPE	CONTENTS
1. 2.	stdin	ASCII BINARY	basic input required to run the water quality model geometry as supplied from the ECOMSED
۷.	gcm_geom	DINANT	hydrodynamic model
3.	wet_grid	BINARY	row, column (I,J) locations of the water segments in the hydrodynamic model
4.	hydfilna	BINARY	transport terms as supplied from the hydrodynamic
			model (this is the ECOMSED gcm_tran file)
5.	dffilna	BINARY	diffuser (or outfall) locations and discharge values as
			supplied from the hydrodynamic model
6	bcfilna	ASCII/binary	boundary condition concentrations for each system
7	psfilna	ASCII/binary	point source loads for each system
8	npsfilna	ASCII/binary	nonpoint source loads for each system
9	flfilna	ASCII/binary	fall-line loads for each system
10	atmfilna	ASCII/binary	atmospheric loads for each system
11	pcfilna	ASCII/binary	model parameters, constants and time-functions as
	p c ······ci	, , , , , , , , , , , , , , , , , , , ,	required by the TUNER kinetic subroutine
12	icfilna	ASCII/binary	initial conditions for each system
13	sedfilna	ASCII	input required for applications involving sediment flux models
			IIIUUGIS

#### **B. MODEL GENERATED OUTPUT FILES**

	<u>NAME</u>	<u>TYPE</u>	CONTENTS
1.	stdout	ASCII	standard output containing all the input information and computed values as selected by the user
2.	RCAF10	BINARY	the system bypass options and times at which the grid-wide dumps were generated
3.	RCAF11	BINARY	a time-history of the grid-wide or global dumps for all state-variables
4.	RCAF12	BINARY	system bypass options, dump variable names and times at which the detailed dumps were generated (for selected segments)
5.	RCAF13	BINARY	a more-detailed time-history dump for selected segments and selected parameters
6.	RCAFIC	BINARY	concentration profiles to be used for multi-year, multi-month, etc. running (provides a "hot start" capability)



#### TABLE 2. RCA FILE STRUCTURE, Continued

7.	RCAF14	BINARY	the concentrations and fluxes computed by the sediment nutrient flux subroutine, if invoked by the user
8.	RCAFICSED	BINARY	concentration profiles for the sediment for multi-year running (provides a "hot start" capability), if the sediment nutrient flux subroutine is invoked by the user
9.	RCAFMB	BINARY	a time history of mass balance and flux balance terms for the water column
10.	RCAFMBSED	BINARY	a time history of mass balance and flux balance terms for the sediment nutrient flux subroutine

Appendix D provides greater detail as to the "structure" of the RCA output files.



### 2.0 RCA Model Input Data Description

The inputs required by RCA have been organized into a number of Input Groups and in turn into a number of input files. Table 3 presents the major input groups and associated files (there is a main input file and a number of associated input files):

TABLE 3. LISTING OF MAJOR INPUTS TO RCA BY GROUP

Input		
<u>Group</u>	<u>File</u>	Description
Α	stdin	model descriptor information
В	stdin	print control and integration history
С	stdin	hydrodynamic time breaks and scale factors
D	stdin	names of data files to be used for the input of: boundary
		conditions; point source loads; nonpoint source loads; fall-
		line loads; atmospheric loads; parameters, constants and
		time functions; and initial conditions
E	stdin	stability and accuracy criteria
F	stdin	end of simulation dumps
G	bcfilna	boundary conditions
Н	psfilna	point source loads
I	npsfilna	nonpoint source loads
J	flfilna	fall-line loads
K	atmfilna	atmospheric loads
L	pcfilna	parameters, constants and time functions
М	icfilna	initial conditions



## GROUP A: MODEL DESCRIPTORS (STDIN)

One of the major changes in the input structure of RCA input files between Version 2 and Version 3 of the model code is that now RCA requires a comment or title record to be placed before all input records. If the user should so choose, he or she may use the comment line to indicate the variables to be read on the following record. See below for an example.

Inputs required for this group include:

- 1. linked run option, model listing options, and model execution options
- 2. model title and run description
- 3. water quality state-variable names
- 4. system by-pass options

#### A1. <u>Linked Run Option, Model Listing Options and Model Execution Options</u>

Com FORMAT (	80 nment A80)	
Comment	=	Comment line (ignored by RCA)
10	20 30	40 50 60 70 80
CYCLE LIS	ST1 LIST2	LIST3 LIST4 LIST5 IDIAGDT INPCHCK
FORMAT(10I	10)	
CYCLE	=	linked run option (permits the user to link sequential or multiple year runs together)  = 0, model grid initial conditions are read from the icfilna input file (this is equivalent to a cold-start)  = 1, model grid initial conditions are read from the RCAFIC file, which has been generated by a previous execution of RCA (this is equivalent to a hot-start)
LIST1	=	geometry (segment volumes) and transport (flow and dispersion) list option
LIST2 LIST3 LIST4 LIST5 LIST#	= = = =	boundary conditions list option loadings list option parameters, constants and time functions list option initial conditions list option = 0, do not list input



= 1, list input

IDIAGDT = execution option

= 0, perform RCA model run

= 1, just run through input deck to determine critical

integration timesteps

INPCHCK = input checker option

= 0, perform RCA model run

= 1, just read through input deck to check for input errors

CYCLE should always be equal to 0 for a user's first run and then may be optionally set equal to 1, if the user is performing multi-year (multi-month, etc.) runs using multiple hydrodynamic transport files (gcm\_tran). In order to reduce disk storage utilization, it is recommended that the user set LIST# equal to 0 unless performing verification of model inputs.

IDIAGDT can be set equal to 1 on the initial model run in order to determine the critical detention time (and, therefore, maximum timestep size for explicit integration) of the model. Should the user select the split-timestep integration algorithm, setting IDIAGDT will provide useful information for setting both critical and regular timestep sizes. Subsequently, the user would set IDIAGDT to 0 in order to perform full model simulations.

The user should set INPCHCK = 1 the first time running a new input deck to permit RCA to identify any input errors. After an input deck is read without errors, the user can set INPCHCK = 0 and proceed to perform a model simulation.

An example of the use of the "Comment" record and actual input record follows:

#### A2. Model Title and Run Description

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

80 TITLE FORMAT (A80)



TITLE = user specified title or run description

The user may specify as many lines as desired for the title and/or run description. This input is terminated when RCA encounters a record with "END" or "end" in columns 1-3. For example:

LISS 3.0 Long Island Sound Study - 3-D Version

Uses NOAA Hydrodynamic Files Received 12/04/90

Algal Growth Rates = 2.0 and 0.9 /day Low Grazing Pressure

Recycle Rates = 0.05 /day Algal settling is a function of nutrient status

Base settling rate = 0.5 m/day - nutrient depleted settling rate = 0.5 m/day

END

#### A3. <u>State-Variable Names</u>

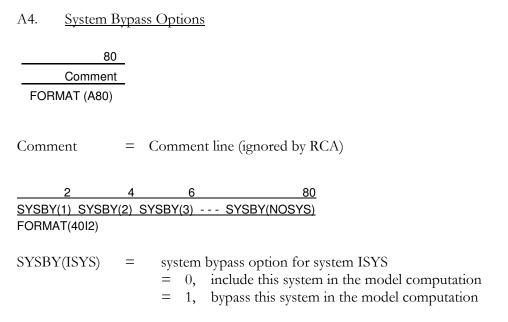
80

FORMAT(10A8)

SYNAME(ISYS) = user specified header to describe system ISYS (NOSYS is the total number of systems or state-variables in the water quality model)

Note: Although these system names are not used explicitly in RCA, they will be used when printing input data associated with loads, boundary conditions, and initial conditions. The order of the system names is determined by the user's kinetic subroutine (TUNER).





The system bypass option permits the user to include or exclude water quality variables from the model computation without performing major revisions to the user supplied inputs. The user should, however, make sure that the TUNER kinetic subroutine is written in such a way as to permit the by-passing or exclusion of the selected state-variables.

# GROUP B: PRINT CONTROL AND INTEGRATION CONTROL INFORMATION (STDIN)

Inputs required for this group include:

- 1. integration solution options,
- 2. time-warp scale factor and start of simulation time,
- 3. number of integration step-sizes,
- 4. integration step-size history,
- 5. global and detailed print intervals and number of segments for detailed dumps,
- 6. segments for which detailed dumps are to be saved,
- 7. intermediate dump segments,
- 8. by-pass options for detailed dumps.
- 9. mass balance/flux balance options

#### B1. <u>Integration Procedure Solution Options</u>

80

Comment	-	
FORMAT (A80)	=	
Comment	=	Comment line (ignored by RCA)
10	20	<u>30 40 50</u>
INTGRTYP NEGS	SLN	SLCOPT ISMOLAR ISMOLBCOPT
FORMAT(5I10)		
INTGRTYP	=	integration procedure to be used for the simulation  = 1, explicit integration algorithm  = 3, split-time step algorithm  = 4, explicit integration using Smolarkiewicz corrector  = 5, leap-frog with Smolarkiewicz corrector  = 6, split-timestep with Smolarkiewicz corrector  (Note: options 3 and 6 are available only in the in-house
NEGSLN	=	version of RCA) option to permit the computation of negative concentrations = 0, restrict concentrations to the positive plane (normal option) = 1, permit the integration procedure to compute negative concentrations - used for special applications such as computing DO deficit or computing pH/alkalinity
SLCOPT	=	<ul> <li>option for sigma-level correction for horizontal diffusion</li> <li>= 0, no corrections will be applied</li> <li>= 1, the sigma-level correction algorithm will be applied when computing horizontal fluxes</li> </ul>



ISMOLAR = option for Smolarkiewicz correction

= 0, use 2<sup>nd</sup> order accurate Smolarkiewicz scheme

= 1, use recursive Smolarkiewicz scheme

ISMOLBCOPT = option for applying Smolarkiewicz correction schemes at

boundaries

= 0, do not apply Smolarkiewicz scheme at boundaries

= 1, apply Smolarkiewicz scheme at boundaries

Normally, the user should select from either the explicit (INTGRTYP = 1 or 4) or the split-timestep algorithms (INTGRTYP=3 or 6) and positive solutions only (NEGSLN=0) options. Generally, by using the split-timestep option, the user can specify bigger timesteps for most segments within the model grid (only integrating a few critical segments with a small timestep) then could be chosen for explicit integration. It is strongly recommended that users not use option 5 for the reasons described previously. Usually either option 4 or 6 should be selected so as to reduce numerical dispersion (but at some cost in computational burden). The user can always evaluate the impact of numerical dispersion by running the model with and without Smolarkiewicz corrections and then comparing runs. For debugging purposes the user may wish to select INTGRTYP=1. When INTGRTYP is set equal to 1, the user may, for a particular segment, directly compute all of the terms of the derivative and compute the expected concentration at the next time level, via Equation 4:

$$c_{i}^{n+1} = c_{i}^{n} + \Delta t \left( \sum Q_{ij} c_{i}^{n} + \sum R_{ij} c_{i}^{n} - \sum \left( Q_{ik} + R_{ik} \right) c_{i}^{n} + W_{i} + K_{i} V_{i} c_{i}^{n} \right)$$
(4)

where superscripts denote time levels in the integration and subscripts denote the model grid cells or segments.

The user should be aware that if NEGSLN is set equal to 0 and RCA computes a negative concentration for a segment (or group of segments) for a time-step, RCA will not let the concentration go negative. Rather, RCA will set the concentration for the next time-step to one quarter of the old concentration. Since this, in effect, results in adding mass to the system, RCA will print a warning message. If the number of occurrences of this corrective action is small and/or the mass being added to the system is small the user should not be too concerned. If, however, the number of warning messages and/or the mass being added to the system is large, the user should rerun the simulation using smaller time-steps for the critical period.

The choice of a value for ISMOLAR should be guided by experience and side-by-side comparisons. Generally use of the recursive version of the Smolarkiewicz corrector (ISMOLAR=1) provides for greater numerical accuracy, but at a cost of 30-50 percent increase in simulation run time. It may be possible to utilize the 2<sup>nd</sup> order accurate form of Smolarkiewicz (ISMOLAR=0) and reduce simulation run times, but the user should perform simulations using both options and compare results to see if the differences between schemes are acceptable.



The choice of applying either Smolarkiewicz correction scheme at the boundary should also be guided by experience and the frequency and quality of boundary condition data. For example, in tidal systems if data are only available on a monthly basis, it is probably better not to use Smolarkiewicz corrections at the boundary. If, however, for a tidal system where boundary conditions can be specified from hourly data (i.e., from continuous recorders) or from another model (as in the case of nested-models) the use of a Smolarkiewicz correction algorithm may be appropriate.

#### B2. <u>Sigma-Level Correction Parameters (SLCOPT = 1)</u>

A sigma-level grid may result in some undesired mixing in regions of steep topography. In some cases where the layers follow the river bottom or sea-bed of the water body, adjacent segments in the same layer can lie at significantly different depths in the vicinity of steep gradients. Because of this, "horizontal" diffusion between adjacent segments can result in an artificial vertical diffusion.

The numerical error caused by this can be reduced by using a correction method based on horizontally averaged concentrations. This method involves calculating the domain averages at user-specified standard depths, and performing horizontal mixing calculations using the divergence from the average instead of the actual concentration.

It is not necessary to specify the surface level (i.e., depth = 0) when specifying the standard level depths. If the surface depth is not specified, constituent values associated with the first sigma level are used for the surface values. To ensure proper interpolation from the standard levels back to the sigma levels, each bottom sigma level must be bracketed by two standard levels, i.e., it is required to specify a standard level depth greater than the maximum expected depth in sigma-level space.

80	
Comment	
FORMAT (A80)	

Comment = Comment line (ignored by RCA)

10	20	30
IDTSLCSECS	TWARPSLC	NOSLC
FORMAT (FI10, 6X,A4,I10)		

IDTSLCSECS = time interval between corrections (days)

TWARPSLC = time-warp or units used for IDTSLC. Normally

IDTSLCSECS is in units of seconds. The user may, however,

use different units.

= SECS or secs

= MINS or mins



NOSLC = number of standard levels

 10
 20
 80

 SLCDPTH(1)
 SLCDPTH(2)
 ⋅⋅⋅ SLCDPTH(NOSLC)

 FORMAT (8F10.0)
 ⋅⋅⋅
 SLCDPTH(NOSLC)

SLCDPTH = standard-level depths

B3. <u>Time Warp Scale Factor, Start of Simulation Time and Integration Interval for</u> Kinetic Subroutine

Comment FORMAT (A80)

Comment | Comment line (ignored by RCA)

10 20 30 TWARP TZERO IDTWQ FORMAT(6X,A4,F10.0,I10)

TWARP = scale factor for integration step-size information. Normally

the units for the general integration step-size, DT, and the kinetics integration step-size IDTWQ are seconds. However, the user may change the units of the input via TWARP.

= SECS or secs, DT and IDTWQ are read in seconds,

= MINS or mins, DT and IDTWQ are read in minutes,

= HRS or hrs, DT and IDTWQ are read in hours.

TZERO = prototype time for start of the simulation (days). Usually

TZERO is set equal to 0.0, however, the user may start the simulation at a time greater than zero. For example, the user may wish to skip computing the winter months of a eutrophication model during the early calibration effort in order to reduce computer requirements. If the user has defined time equal to zero as January 1st and wishes to start the simulation in early May, TZERO would be set equal to 120. RCA would then ensure that all time-dependent inputs are at their proper starting values before initiating the

simulation.

IDTWQ = integration interval for the kinetic subroutine (nominally in

seconds). If IDTWQ = 0, RCA will integrate the kinetic portion of the derivative at the same timestep as used for the transport (see Card Group B4 below). If IDTWQ> 0, then the kinetic subroutine, TUNER, will be called every IDTWQ

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seconds. The latter implies that the kinetic portion of the derivative is assumed to be constant over the interval IDTWQ. (Note: the user should ensure that the value chosen for IDTWQ should be an exact multiple of any value of ISTEP or IDTSPLIT - see below).

The following inputs (B4 and B5) are required for INTGRTYP = 1, 4 or 5

### B4. Number of Integration Step-Sizes (INTGRTYP = 1, 4, or 5)

For a number of water quality problems, there may be periods of time within the simulation period for which small integration steps are required (ex. during storm runoff events or spring snowmelt) versus times when larger timesteps can be used (ex. summer low flow). Therefore, RCA permits the user to specify a time-variable history of integration stepsizes to be used during the simulation.

Commer FORMAT (A80)	nt_					
Comment	=	Comme	ent line (igr	nored by RC	ZA)	
NSTEP FORMAT(I10)						
NSTEP	=	number	of integra	tion step-siz	es to be read	
B5. <u>Integrat</u>	ion Ste	ep-Size Hi	istory (INT	GRTYP =	1, 4, or 5)	
Comme FORMAT (A80)						
Comment	=	Comme	ent line (igr	nored by RC	ZA)	
10 ISTEP(1) TBRK	20 1) IST	30 EP(2) TB	40 RK(2)I		70 P) TBRK(NST	<u>80</u>

integration step-size (seconds)

switching to ISTEP(I+1) until TBRK(I+1)

time (days) until which ISTEP(I) is to be used, then



ISTEP(I)

TBRK(I)

The default units for ISTEP are seconds. However, if TWARP is specified as minutes, hours, or days then values for ISTEP will be in the same units as specified by TWARP. (Note: the value of ISTEP(I) should be an exact divisor of TBRK(I) for each ISTEP/TBRK pair and all ISTEP/TBRK pairs must be an exact divisor of IHYDDT-see C2 below).

The following input (B6) is required for INTGRTYP = 3 or 6

B6. <u>Integration Stepsizes and Total Simulation Time (INTGRTYP = 3 or 6)</u>

Comment FORMAT (A80)

Comment ine (ignored by RCA)

10 20 30 IDTSPLIT IDTFULL TEND

FORMAT (2I10,F10.0)

IDTSPLIT = timestep to be used for the "high speed" or "critical" timestep

segments (seconds)

IDTFULL = timestep to be used for remaining segments (seconds)

TEND = total simulation time, in days

The default units for IDTSPLIT and IDTFULL are seconds. However, if TWARP is specified as minutes, hours, or days then values for IDTSPLIT and IDTFULL will be in the same units as specified by TWARP. (Note: IDTSPLIT should be an exact divisor of IDTFULL and both IDTSPLIT and IDTFULL need to be an exact divisor of IHYDDT - see C2 below).

#### B7. Print Control Information

RCA permits two types of output dumps to be generated: global or domain-wide dumps at "coarse" time intervals, and detailed or selected segments at "fine" time intervals. By global dumps it is meant that the concentrations of all systems for all segments (i.e. all x, y, and z) are saved at the print interval, IPRNTG, described below. A note of caution: if a user has a 100 x 100 grid with 10 depth levels and 25 systems, a total of 10 Mbytes will be written at every IPRNTG interval. Clearly, one should not generate global dumps every day for a one year simulations (unless one has a disc storage system with large capacity).

However, in order to permit the user to generate daily (or hourly) output if necessary an option has been included in RCA to permit the user to select a number of segments



for which information will be stored at a finer interval, IPRNTD, than is used for global dumps.

Comment FORMAT (A80)

Comment | = Comment line (ignored by RCA)

_	10	20	30	40	50	60
	IPRNTG	IPRNTD	NDMPS	TWARPP	IGDOPT	IDDOPT

FORMAT (3I10,6X,A4,2I10)

IPRNTG = time interval (default = seconds) for saving "global" (or grid-wide) concentrations,

IPRNTD = time interval (default = seconds) for saving "detailed" (or segment specific) concentrations and rate terms as per the user

kinetic subroutine,

NDMPS = number of selected segments to be used in generating detailed

dumps if IPRNTD≠0

TWARPP = units in which IPRNTG and IPRNTD are input. Acceptable

units for IPRNTG and IPRNTD are SECS (seconds), MINS (minutes), HRS (hours), or DAYS (days) and may be entered in

either upper or lower case.

So, for example, a user who wished to get detailed dumps at one day intervals could specify IPRNTD = 86400, TWARPP =

SECS or IPRNTD = 1, TWARPP = DAYS.

IGDOPT = global dump averaging option

= 0, write instantaneous (i.e., no averaging) concentrations or

rates

= 1, write "averaged" concentrations or rates, using

IPRNTG as the averaging interval

IDDOPT = detailed dump averaging option

= 0, write instantaneous (i.e., no averaging) concentrations or

rates

= 1, write "averaged" concentrations or rates, using

IPRNTD as the averaging interval

B8. <u>Segments for which Detailed Dumps are to be saved</u>

(Note: if IPRNTD = 0 or NDMPS = 0) skip this group and continue with B9.)



Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

4 8 12 72

IFDMPS(1,1) IFDMPS(1,2) IFDMPS(1,3) --- IFDMPS(NDMP,3)

FORMAT (1814)

IFDMPS(I,1) = X, Y and Z location designations, respectively, for the desired segments to be saved

IFDMP(I,2) segments to be saved

B9. System Bypass Options for Detailed Dumps

DDMPBY(ISYS) =

Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

2 4 80

DDMPBY(1) DDMPBY(2) --- DDMPBY(NOSYS)

FORMAT(40I2)

system bypass options for making detailed dumps
0, include this system when making detailed dumps
1, do not include this system when making detailed dumps

This option permits the user to generate detailed dumps for a system even if that system is being bypassed (SYSBY=1) in the overall model computation. The major reason for including this option is so that users do not need to modify their GDP command decks if systems on being turned on and off during the calibration process. Of course, the user can also bypass making detailed dumps for a system (by setting DDMPBY=1), even if the system is being computed. However, the user should be sure to check whether the kinetic subroutine TUNER has been written in such a way as to make this input option function properly.

#### B10. Segments to be Displayed for Intermediate Dumps

RCA permits the user to monitor the progress of the water quality simulation by dumping the concentrations of six segments to the screen (or the user's output file with



access via the UNIX/LINUX "tail" command) at each print interval during the simulation.

Comment FORMAT (A80)

Comment | = Comment line (ignored by RCA)

4 8 12 16 20 24 64 68 72 IX (1) IY(1) IZ(1) IX (2) IY(2) IZ(2) --- IX (6) IY(6) IZ(6) FORMAT(18I4)

IX,IY,IZ = X, Y and Z IDs of segments to be displayed during the simulation.

B11. Mass Balance - Mass Flux Computation Options

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

 10
 20
 30
 40
 50
 60

 MASSBAL
 IPRNTMB
 TWARPMB
 IMBOPT
 ISTARTMB
 IENDMB

FORMAT (2I10,6X,A4,3I10)

MASSBAL = mass/flux balance computation option

= 0, do not perform mass or flux balance computations

= 1, perform mass and flux balance computations

IPRNTMB = print interval (default = seconds) for saving mass balance and

flux balance computations

TWARPMB = units in which IPRNTMB, ISTARTMB, and IENDMB are

input. Acceptable units are SECS (seconds), MINS (minutes),

HRS (hours), or DAYS (days).

IMBOPT = mass/flux balance dump averaging option

= 0, dump instantaneous (i.e., no averaging) mass balance

and flux balance computations

= 1, dump "averaged" mass balance and flux balance computations, using IPRNTMB as the averaging

interval



ISTARTMB = starting time (default = seconds) for beginning mass

balance/flux balance computations

IENDMB = ending time (default = seconds) for performing mass

balance/flux balance computations

This option permits the user to perform domain-wide mass/flux balance computations. The model output can be used to assess the importance of boundary inflows/outflows versus point, non-point, and atmospheric inputs, as well as to perform system-wide mass balance checks.

When selecting a "print interval" for applications in estuarine systems, it is recommended to select a print interval that is an exact multiple of a tidal cycle (44712 seconds or 12.42 hours). If one selects a non-tidal print interval it may make interpretation of flux balance results more difficult since the model would be outputting flux balances that occur over different parts of the tidal cycle and thus, for example, on a flood tide the model output would reflect a net import of mass into the model domain, while output on an ebb tide would reflect a net export of mass from the model domain. It is possible then in a tidal system where there is a small net export of mass from the domain that the flux balance would show a net import of mass if one were to start the flux balances at mean tide or mean tidal elevation but end the simulation at maximum flood tide. The user can also specify the starting and ending times, ISTARTMB and IENDMB, respectively, to help overcome this potential problem. (Example: if one were to perform a 365 day simulation, one could set ISTARTMB = 0 and then specify IENDMB = 31521960 seconds = 364.8375 days and the model will end at the same point in the tidal cycle.)



## GROUP C: HYDRODYNAMIC TIME BREAKS AND SCALE FACTORS (STDIN)

Inputs required for this group include:

- 1. hydrodynamic file input options
- 2. time breaks for the hydrodynamic fields
- 3. flow and dispersion scale factors
- 4. file name containing the ECOMSED hydrodynamic fields

### C1. <u>Hydrodynamic File Input Options</u>

80	
Comment	
FORMAT (A80)	
Comment	= Comment line (ignored by RCA)
10	20 30 40
ICOLLOPT HYDCY	COPT_LNDWTROPTIDIFFOPT_
FORMAT(4I10)	
ICOLLOPT :	option to inform RCA whether the gcm-geom and gcm_tran have been grid collapsed (i.e., the water quality model is a collapsed or aggregated version of the hydrodynamic grid)
HYDCYCOPT :	<ul> <li>= 0, no grid collapse was performed</li> <li>= 1, grid collapse was performed</li> <li>option to permit RCA to "cycle" or repeat the "gcm_tran" file,</li> <li>i.e. hydrodynamics are at periodic steady-state</li> <li>= 0, do not "cycle" hydrodynamics if end-of-file encountered</li> </ul>

LNDWTROPT = option to select whether full-grid (land/water) hydrodynamic input to be read or just water cells

= 0, full-grid, i.e., land and water

= 1, just water cells (requires "wet-grid" input file from ECOMSED)

"cycle" hydrodynamics, i.e., go back to beginning of the hydrodynamic file if end-of-file encountered

IDIFFOPT = option to specify and read "diffuser" files generated by ECOMSED

= 0, no diffuser files specified

= 1, diffuser files will be specified

The use of the HYDCYCOPT options permits users to perform water quality simulations for periods of time longer than the hydrodynamic model was run. For



example, suppose a user wanted to run a 10 day simulation of a dye release into a tidal creek, subject to no freshwater inflow and with a constant tidal amplitude. The user could run the hydrodynamic model and save 10 days of periodic stage and velocity and set HYDCYCOPT = 0, or just run the hydrodynamic model for one tidal cycle and save just one tidal cycle worth of stage and velocity and set, HYDCYCOPT = 1. RCA would go back to the beginning of the gcm\_tran file (recycle) when the simulation time reached tidal cycle 1, 2, (day) etc. (Note: The use of HYDCYCOPT = 1 assumes that the hydrodynamics are at periodic steady-state.)

### C2. <u>Time Breaks for the Hydrodynamic Fields</u>

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 20 IHYDDT UNITS FORMAT(I10,6X,A4)

IHYDDT = averaging period used by ECOMSED to save hydrodynamic

output (nominally in secs).

UNITS = time-warp or units used for IHYDDT. Normally IHYDDT

is input in units of seconds. The user may, however, use

different units:

= SECS or secs, IHYDDT is read in seconds,

= MINS or mins, IHYDDT is read in minutes,

= HRS or hrs, IHYDDT is read in hours.

#### C3. <u>Dispersive Scale Factors</u>

Comment FORMAT (A80)

Comment | = Comment line (ignored by RCA)

10 20 30

SCALRX SCALRY SCALRZ

FORMAT(3F10.0)

SCALRX = scale factor to multiply all horizontal or x-direction dispersion

coefficients by



SCALRY = scale factor to multiply all lateral or y-direction dispersion

coefficients by

SCALRZ = scale factor to multiply all vertical or z-direction dispersion

coefficients by

Normally, SCALRX, SCALRY and SCALRZ should be set equal to 1.0.

C4. The Number of Hydrodynamic and Diffuser Files

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

NOHYDFILNA
FORMAT (I10)

NOHYDFILNA = number of hydrodynamic and diffuser (if supplied by ECOMSED) files to be used in this simulation (maximum of 36)

C5. The Names of the Files Containing the Hydrodynamic and Diffuser Transport Fields

Comment FORMAT (A80)

Comment | = Comment line (ignored by RCA)

40 80
HYDFILNA DIFFILNA
FORMAT(2A40)

HYDFILNA =

complete path length and file name containing the ECOMSED transport and surface elevation data (gcm\_tran)

ex.1 /usersb/neng0010/HYDRO/gcm\_tran

ex.2 ../HYDRO/hydro.84 ex.3 ../HYDRO/hydro.85

(Note: the use of a "/" to specify the path or directory structure for a file is consistent with UNIX or



LINUX file naming structure. Running RCA under a WINDOWS environment means, of course (thanks to Bill Gates), using "\".

DIFFILNA =

complete path length and file name containing the ECOMSED diffuser (or outfall) discharge information (gcm\_gdiff).



## GROUP D: INPUT FILE NAMES (STDIN)

Inputs required for this group include:

- 1. the name of the file to be used to read boundary conditions inputs
- 2. the name of the file to be used to read point source loading inputs
- 3. the name of the file to be used to read nonpoint source loading inputs
- 4. the name of the file to be used to read fall-line loading inputs
- 5. the name of the file to be used to read atmospheric loading inputs
- 6. the name of the file to be used to read parameters, constants, miscellaneous time-variable functions and file names of miscellaneous files required by the users kinetic subroutine
- 7. the name of the file to be used to read initial conditions

RCA has been programmed so as to permit the user to develop a number of subfiles that contain RCA required inputs, rather than have all of the model input contained in one large input file as is done in AESOP. The reason for this is to provide the user with an extra degree of flexibility in generating model input files. If, for example, the user wishes to evaluate model response to a specific waste discharger, the user can set up two point source loading files, one with the discharger's load included and one with it not included. The user would then edit the standard input (STDIN) file and change the file name associated with the point source loadings (specified by D2) to the appropriate external point source file and then execute RCA. Since the standard input file (consisting of various input options for integration and printout histories and file names for the aforementioned RCA inputs) is so small, the time spent in editing should be very short. In addition, having various input groups permits users to develop a number of utility programs to generate the relevant input files rather than have one large complicated program to generate the entire input file at one time.

Further, as an option, the boundary condition, point source, etc. files may be read in either ASCII or binary (to save disc space) format. Binary format, of course, means that another FORTRAN program or utility must be used to generate the file. For binary files the user SHOULD NOT include the "comment" records in his or her input file.

New to RCA 3.0 is the option to bypass a particular file by specifying "NULL" or "null" (without the quotes) in the first four spaces. For example, if a particular application has no fall-line loads, the user just has to specify "NULL" for FLFILNA instead of having to create a dummy fall-line loads file with no loads.



D1. The Name of the File to be Used to Read Boundary Conditions Inputs, Binary Read Option

Comment FORMAT (A80)

Comment | = Comment line (ignored by RCA)

40 50 BCFILNA IBNRYOPT FORMAT(A40, I10)

BCFILNA = complete path length and file name containing the boundary condition information (i.e., boundary segments and concentrations)

ex.1 /usersb/neng0010/HYDRO/boundcond (input file named "boundcond" resides in the /usersb/neng0010/HYDRO directory)

ex.2 bc.file (input file name bc.file resides in the current directory)

ex.3 ../inputs/bc.84 (input file named bc.84 resides in the inputs directory, which is a subdirectory of the directory one level above the currect directory

NULL to bypass this file. The appropriate vectors will be set to zero.

IBNRYOPT = option telling RCA to read ASCII or binary formatted boundary condition file

= 0, read ASCII file

= 1, read binary file

D2. The Name of the File to be Used to Read Point Source Loading Inputs, Binary Read Option

Comment FORMAT (A80)

Comment ine (ignored by RCA)

PSFILNA IBNRYOPT FORMAT(A40,I10)



PSFILNA = complete path length and file name containing the point

source loading information (loading segments and point

source loads)

= NULL to bypass this file. The appropriate vectors will be set

to zero.

IBNRYOPT = option telling RCA to read ASCII or binary formated file

= 0, read ASCII file

= 1, read binary file

# D3. The Name of the File to be Used to Read Nonpoint Source Loading Inputs, Binary Read Option

Comment FORMAT (A80)

Comment | = Comment line (ignored by RCA)

40 5

NPSFILNA IBNRYOPT

FORMAT(A40,I10)

NPSFILNA = complete path length and file name containing the nonpoint

source loading information (loading segments and nonpoint

source loads)

NULL to bypass this file. The appropriate vectors will be set

to zero.

IBNRYOPT = option telling RCA to read ASCII or binary formated files

= 0, read ASCII file

= 1, read binary file

## D4. The Name of the File to be Used to Read Fall-line Loading Inputs, Binary Read Option

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

40 50

FLFILNA IBNRYOPT

FORMAT(A40,I10)



FLFILNA = complete path length and file name containing the fall-line

loading information (fall-line segments and fall-line loads)

NULL to bypass this file. The appropriate vectors will be set

to zero.

IBNRYOPT = option telling RCA to read ASCII or finary formatted file

= 0, read ASCII file = 1, read binary file

D5. The Name of the File to be Used to Read Atmospheric Loading Inputs, Binary Read Option

80 Comment

FORMAT (A80)

Comment | Comment line (ignored by RCA)

40 50

ATMFILNA IBNRYOPT FORMAT(A40,I10)

ATMFILNA = complete path length and file name containing the

atmospheric loading information (amtospheric loads)

= NULL to bypass this file. The appropriate vectors will be set

to zero

IBNRYOPT = option telling RCA to read ASCII or binary formated file

= 0, read ASCII file

= 1, read binary file

D6. The Name of the File to be Used to Read Parameters, Constants, Time-Variable Functions and Miscellaneous File Names, Binary Read Option

80 Comment

FORMAT (A80)

Comment | Comment line (ignored by RCA)

40 50

PCFILNA IBNRYOPT FORMAT(A40,I10)

**PCFILNA** 

complete path length and file name containing the parameters,

constants and time-variable functions



= NULL to bypass this file. The appropriate vectors will be set to zero.

IBNRYOPT = option telling RCA to read ASCII or binary formatted files

= 0, read ASCII file= 1, read binary file

D7. The Name of the File to be Used to Read Initial Conditions, Binary Read Option

Comment FORMAT (A80)

Comment | Comment line (ignored by RCA)

40 50 ICFILNA IBNRYOPT FORMAT(A40,I10)

ICFILNA = complete path length and file name containing the initial

conditions

IBNRYOPT = option telling RCA to read ASCII or binary formatted files

= 0, read ASCII file= 1, read binary file



## GROUP E: STABILITY AND ACCURACY CRITERIA (STDIN)

E1. Stability Criteria

Comment FORMAT(A80)

Comment ine (ignored by RCA)

20 30 80 CMAX(1) CMAX(2) --- CMAX(NOSYS)

FORMAT(10X,7F10.0)

CMAX(ISYS) =

stability criteria for system ISYS, i.e. a maximum concentration that if exceeded in any segment or grid cell indicates that the numerical integration procedure has become unstable. If an instability occurs an appropriate error message is written and the simulation is terminated.

### E2. <u>Minimum Concentrations for Numerical Integration</u>

Comment FORMAT (A80)

Comment | Comment line (ignored by RCA)

20 30 80

CMIN(1) CMIN(2) - - - CMIN(NOSYS)

FORMAT(10X,7F10.0)

CMIN(ISYS) =

the minimum concentration or "floor" for system ISYS. As was mentioned earlier, under the description of the input variable NEGSLN, RCA normally does not permit negative solutions to occur. It does this by "quartering" concentrations. If, however, enough "quartering" of concentrations occur in a segment, underflows (i.e., concentrations less than 1.0E-38) may occur, which will result in the RCA run terminating. To prevent this the user should specify minimum values which will limit the "quartering" process. Recommended values for CMIN are 1.0E-20.



## GROUP F: END OF SIMULATION DUMPS (STDIN)

Inputs from this group are read at the end of a simulation run.

### F1. System Dumps

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

At the completion of the simulation the user may wish to display or dump the concentrations of any or all segments for any or all systems. The following inputs are read for each global dump saved starting with the first and going through system dump = NGDMP (where NGDMP is set in the users kinetic subroutine).

3	6	9	12	69	72	75	78	80
IVAR	IX(1)	IY(1)	IZ(1)	 IX(8)	IY(8)	IZ(8)	LYRDMP	LYR
FORM	AT(I3	,2413,	43,I2)					

IVAR = 1, for global system dumps (Note: currently only the state-variable concentrations are available for dumping, hence IVAR = 1. However, in the future, RCA may permit IVAR may take on other values.)

IX,IY,IZ = x, y and z designation for the segment to be displayed

LYRDMP = if LYRDMP is read in as "LYR" then all segments within a particular layer (for layer = LYR) will be displayed without the user being required to specify each IX,IY,IZ combination

LYR = the layer for which concentrations are to be dumped (if

LYRDMP is read as "LYR")

Table 4 presents an example of the STDIN input file for Groups A through F.



#### TABLE 4. EXAMPLE OF STANDARD INPUT FILE - STDIN

```
Cycle List_Geom List_BCs List_WKs List_PCs List_ICs IDIAGDT 0 0 0 0 0
                                                                                                                                                                          INPCHK
          Model Run Descriptor Comments Follow (Terminate with an "END")
    MERL Tank Simulation
     Input set up to simulate Control Tanks 0 - 5 - 8
END
           System Names (1 ... NOSYS)
SAL PHYT1 PHYT2 RPC
                                                                RPÓP
                                                                                                                        T<sub>1</sub>DOP
                                                                                                                                             DTP
          RDON
                           LDON
                                               NH3
                                                                 NO23
                                                                                     SIU
                                                                                                          SI
                                                                                                                        RPOC
                                                                                                                                          LPOC
                                                                                                                                                             RDOC
                                                                                                                                                                                LDOC
                                              02EQ
       REDOC
                       EXDOC
                                                                  DΩ
C Type of Simulation
TIME-VARIABLE SIMULATION
TZERO IDTWQSECS
            TWARP
              MTNS
                                       0.0
            NSTEP
CIntg_Step UntilTime Intg_Step UntilTime Intg_
                240
                                       240
                                                                                 HRS
  С
C
                                                                                                                    2 2 IENDMB
                                                                                                              0 31521960
1 447120 SECS
C ICOLLOPT HYDCYCOPT LNDWTROPT
                                                                               non-collapsed, non-split hydro files, water only
          IHYDDT
                                   UNITS
                720
                                      HRS
                             SCALRY
                                                    SCALRZ
С
          SCALRX
                 1.0
                                       1.0
                                                          1.000
C
         Number and Names of Hydrodynamic Files
gcm_tran_1-6
gcm_tran_7-12
C Boundary
           Boundary Condition File Name
                                                                                        Binary Read Option
bc058.inp
          Point Source Loads File Name
                                                                                          Binary Read Option
          Non-point Source Loads File Name Binary Read Option
NULL
           Fall-line Loads File Name
                                                                                          Binary Read Option
C Atmospheric Loads File Name
                                                                                          Binary Read Option
            Params, Consts, TVFs File Name
                                                                                         Binary Read Option
pctvf058.inp
           Initial Conditions File Name
                                                                                          Binary Read Option
 ic058.inp
            Stability Concentrations
                                                                              3000.0
stability
                                                                                                                          100.000 500.0
                                   5000. 3000.
.00.00 500.0
                                                                                                     1000.0
                                                                                                                                                    20.0
                                                                                                                                                                             50.00
                                100.00
                                                                              100.00
                                                                                                                                                                           1000.0
                                 1000.0
                                                       1000.0
                                                                              1000.0
                                1000.0
                                                       3000.0
                                                                              5000.0
          floor
         Selection of Simulation Dumps Follow
                                                                                                                                                                      LYR 1
LYR 2
     1
                                                                                                                                                                               End Sys 1
                                                                                                                                                                       LYR
                                                                                                                                                                               1 2
     1
                                                                                                                                                                      LYR
                                                                                                                                                                               End Sys 2
```



## GROUP G: BOUNDARY CONCENTRATIONS (BCFILNA)

The user may choose to input boundary condition information using either sigma-level specification or standard-level specification. For sigma-level specification the user enters the boundary concentrations associated with each boundary segment in the model, specifying both the (IX,IY,IZ) segment location and the average water column concentration at the appropriate model segment depth. For example, assume one is modeling a river with one upstream and one downstream boundary, using a one column wide (i.e. laterally averaged) grid and five equally spaced vertical layers. Then the model has a total of ten boundary conditions, one boundary condition for each of the five upstream layers and one for each of the five downstream layers. If the total depth of the upstream boundary is 5 meters, then the boundary conditions would be assumed to represent water quality conditions every one meter in depth. If the total depth at the downstream boundary is 15 meters, then the boundary conditions would be assumed to represent water quality conditions every three meters in depth.

For standard level specifiation, the user first specifies the standard levels (or depths) at which the boundary conditions will be provided for a particular system and then specifes for each (IX,IY) boundary location the number of standard level depths for this location and the associated water column concentrations at the standard levels or depths. RCA will then interpolate (using linear interpolation) the specified standard level boundary conditions onto the sigma-level grid. Using the same river system model as above, and having water column observations only at the surface, 3 meter, 10 meter and 15 meter depths, the user would specify four standard level depths, i.e. 0, 3, 10 and 15 meters, and two boundary (IX,IY) locations (i.e., the (IX,IY) locations of the upstream and downstream boundaries). For the upstream boundary, data are available for only two standard levels, 0 and 3 meters, while for the downstream boundary the user would input water quality concentrations at the four standard levels, 0, 3, 10 and 15 meters. RCA would then interpolate the two upstream concentrations, using linear interpolation, to equivalent sigma-level depths of 0.5, 1.5, 2.5, 3.5 and 4.5 meters, and would also interpolate the four downstream concentrations onto the downstream sigma-level depths of 1.5, 4.5, 7.5, 10.5, and 13.5 meters.

Inputs required for this group include:

- 1. boundary condition input options
- 2. number of boundary conditions
- 3. scale factor for boundary concentrations
- 4. actual boundary concentrations



## G1. Boundary Condition Input Option

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 20 IBCOPT IBCPWLOPT FORMAT(2I10)

IBCOPT = input option

= 1, time-invariant (or constant) sigma-level concentrations will be read

= 2, time-variable sigma-level boundary concentrations will be read

= 3, time-invariant (or constant) standard level concentrations will be read

 4, time-variable standard level boundary concentrations will be read

IBCPWLOPT =

option to select step-function or piecewise linear interpolation of time-variable boundry conditions.

= 0, step-function interpolation will be used

= 1, piecewise linear interpolation will be used

The remaining boundary condition input is dependent upon the IBCOPT input option chosen. Data inputs for sigma-level option 1 (constant concentrations) and option 2 (time-variable) will be presented first, followed by data inputs associated with standard level options 3 (constant concentrations) and option 4 (time-variable).

#### Constant or Time-Invariant Concentrations - Sigma Level (IBCOPT = 1)

Data associated with Data Types G2, G3 and G4 will be read NOSYS times; once for each system in the model.

#### G2. Number of Boundary Conditions

Comment FORMAT (A80)

Comment | Comment line (ignored by RCA)



NOBC(ISYS) FORMAT(I10) the number of boundary conditions for system ISYS NOBC(ISYS) =(Note: If there are no boundary conditions to be specified for a system (NOBC = 0) then no input is required for G3 or G4; just continue with next G2.) G3. Boundary Concentration Scale Factor 80 Comment FORMAT (A80) Comment Comment line (ignored by RCA) 10 SCALBC(ISYS) FORMAT(F10.0) SCALBC(ISYS) =scale factor for system ISYS Normally SCALBC(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in boundary inputs, SCALBC(ISYS) would then be set equal to 0.75. G4. Boundary Segments and Boundary Concentrations 80 Comment FORMAT (A80) Comment Comment line (ignored by RCA) BBC(1,ISYS) IBC(1,1,ISYS) IBC(2,1,ISYS) IBC(3,1,ISYS) ---74 70 BBC(NOBC,ISYS) IBC(1,NOBC,ISYS) IBC(2,NOBC,ISYS) IBC(3,NOBC,ISYS) FORMAT(4(F10.0,1X,3I3))

boundary concentration (mg/L)

x-cell number of boundary condition grid element



BBC(I,ISYS)

IBC(1,I,ISYS) =

IBC(2,I,ISYS) = y-cell number of boundary condition grid element IBC(3,I,ISYS) = z-cell or layer number of boundary condition grid element

The following example illustrates how to assign the x, y and z information required for RCA.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L
2	L	OWB			L	L	L						L	L	L
3	L	OWB								L				FFI	L
4	L	OWB								L	L			L	L
5	L	OWB											L	L	L
6	L	L	L	L	L	L	L	L	FFI	L	L	L	L	L	L

The above illustration shows a 15x6 grid; NX=15 and NY=6. Grid elements denoted by an "L" indicate either a land segment or the limits of the model domain. Grid elements denoted by "OWB" indicate an open water boundary (including flow and dispersion consistent with the ECOMSED grid notation), while those represented by "FFI" represent free flowing inputs (flow only, no dispersion), such as a river/dam or an onshore outfall/intake discharge. The model also has 6 vertical layers.

The model, then, has 36 ((4 OWB + 2 FFI)\*6) boundary conditions, specified as follows:

IBC(2,I,ISYS)	IBC(3,I,ISYS)
2	1
2	2
:	:
2	6
3	1
:	:
3	6
4	1
:	:
4	6
5	1
:	:
5	6
6	1
:	:
6	6
3	1
:	:
3	6
	2 2 3 3 : 3 4 : 4 5 : 5 6 : 6 3 :



<u>Time-Variable Concentrations - Sigma Level (IBCOPT = 2)</u>

G2. Time for which Boundary Concentrations are being Specified

Comment FORMAT (A80)

Comment | = Comment line (ignored by RCA)

20 30

NXBCTSECS TWARPBC

FORMAT (10X,I10,6XA4)

NXBCTSECS = time in seconds (or units specified by TWARPBC)

TWARPBC = time-warp or units used for NXBCTSECS.

Normally NXBCTSECS is input in units of seconds. The user

may, however, use different units.

= SECS or secs,

= MINS or mins,

= HRS or hrs,

= DAYS or days.

Data associated with Data Types G3 through G6 will be read NOSYS times; once for each system in the model.

G3. Number of Boundary Conditions

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

NOBC(ISYS) FORMAT(I10)

NOBC(ISYS) = the number of boundary conditions for system ISYS

(Note: If there are no boundary conditions to be specified for a system (NOBC = 0), then no input is required for G4, G5 or G6; just continue with next G3.)



G4. <u>Boundary</u>	Concentration Scale Factor
Comment FORMAT (A80)	
Comment	= Comment line (ignored by RCA)
10 SCALBC(ISYS) FORMAT(F10.0)	
SCALBC(ISYS)	= scale factor for system ISYS
2	C(ISYS) would be set equal to 1.0, however, if the user wished to ty run to a 25 percent reduction in boundary inputs, SCALBC(ISYS) equal to 0.75.
G5. <u>Boundary</u>	<u>Segments</u>
Comment FORMAT (A80)	
Comment	= Comment line (ignored by RCA)
14 IBC(1,1,ISYS) IBC(2	17 20 2,1,ISYS) IBC(3,1,ISYS)
<u> </u>	74 77 <u>80</u>
IBC(1,NOBC,ISY) FORMAT(10X,7(I4,I3	S) IBC(2,NOBC,ISYS) IBC(3,NOBC,ISYS) 3,I3))
IBC(2,I,ISYS)	<ul> <li>x-cell number of boundary condition grid element</li> <li>y-cell number of boundary condition grid element</li> <li>z-cell or layer number of boundary condition grid element</li> </ul>
G6. <u>Boundary</u>	<u>Concentrations</u>
20	30 80
BBC(1,ISYS) BBC(2)	2,ISYS) BBC(NOBC(ISYS),ISYS)
FUBIVIA I LIUX /FIU	.U1



BBC(I,ISYS) = boundary concentration (mg/L)

The boundary concentrations (BBC) should be specified in the same order as the x, y, and z (IBC) designations were read. After input types G3 through G6 are repeated for each system, then the simulation time at which the next set of boundary concentrations is to be read, NXBCT, is specified; followed by the next set of boundary concentrations (input type G6); it is not necessary to repeat input types G3, G4 and G5. If NOBC(ISYS) = 0 for system ISYS then the user would skip specifying G6 input data for that system.

Data associated with Data Types G3, G4, G5 and G6 will be read NOSYS times; once for each system in the model.

Constant or Time-Invariant Concentrations - Standard Level (IBCOPT = 3)

## G2. Number of Boundary Conditions

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

NOBC(ISYS) FORMAT(I10)

NOBC(ISYS) = the number of boundary conditions for system ISYS

(Note: If there are no boundary conditions to be specified for a system (NOBC = 0), then no input is required for G3, G4, G5, G6 or G7; just continue with next G2.)

#### G3. Boundary Concentration Scale Factor

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

SCALBC(ISYS) FORMAT(F10.0)



SCALBC(ISYS) = scale factor for system ISYS

Normally SCALBC(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in boundary inputs, SCALBC(ISYS) would then be set equal to 0.75.

## G4. Number of Standard Level Depths

Comment FORMAT (A80)

Comment | = Comment line (ignored by RCA)

5 NLVLS(ISYS) FORMAT(I5)

NLVLS(ISYS) = the maximum number of standard level depths required for

system ISYS

### G5. Standard Level Depths

Comment FORMAT (A80)

Comment ine (ignored by RCA)

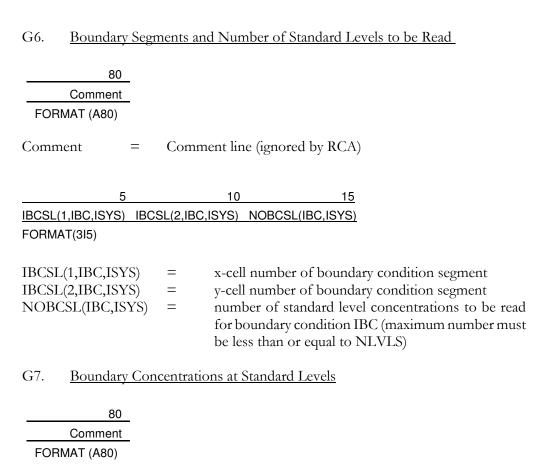
20 30 80

SLDEPTH(1,ISYS) SLDEPTH(2,ISYS) --- SLDEPTH(NLVLS,ISYS)

FORMAT(10X,7F10.0)

SLDEPTH(I,ISYS) = the depth of standard level I, (meters) to be used to specify boundary concentration data for system ISYS





Comment = Comment line (ignored by RCA)

20 30 80

<u>SLBC(1,IBC,ISYS)</u> <u>SLBC(2,IBC,ISYS)</u> — <u>SLBC(NOBCSL,IBC,ISYS)</u> FORMAT(10X,7F10.0)

SLBC(I,IBC,ISYS) = boundary concentration (mg/L)

After reading in the boundary concentrations at the standard levels RCA will perform a linear interpolation of the input data onto the sigma level grid and produce a set of boundary segment numbers (IX,IY and IZ) and concentrations similiar to the input required for IBCOPT = 1.

Inputs G4, G5, G6, and G7 will be read NOBC(ISYS) times; once for each boundary condition



<u>Time-Variable Conditions - Standard Level (IBCOPT = 4)</u>

G2. Time for which Boundary Concentrations are being Specified

Comment FORMAT (A80)

Comment ine (ignored by RCA)

20 30

NXBCTSECS TWARPBC

FORMAT (10X, I10,6X,A4)

NXBCTSECS = time in seconds (or units specified by TWARPBC)

TWARPBC = units to be used for NXBCTSECS

= SECS or secs,= MINS or mins,= HRS or hrs,= DAYS or days.

Data associated with Data Types G3 through G8 will be read NOSYS times; once for each system in the model.

G3. Number of Boundary Conditions

Comment FORMAT (A80)

Comment ine (ignored by RCA)

10 NOBC(ISYS) FORMAT(I10)

NOBC(ISYS) = the number of boundary conditions for system ISYS



(Note: If there are no boundary conditions to be specified for a system (NOBC = 0), then no input is required for G4 to G8; just continue with next G3.)

## G4. Boundary Concentration Scale Factor

Comment FORMAT (A80)

Comment ine (ignored by RCA)

SCALBC(ISYS) FORMAT(F10.0)

SCALBC(ISYS) = scale factor for system ISYS

Normally SCALBC(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in boundary inputs, SCALBC(ISYS) would then be set equal to 0.75.

### G5. Number of Standard Level Depths

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 NLVLS(ISYS) FORMAT(I10)

NLVLS(ISYS) = the maximum number of standard level depths required to

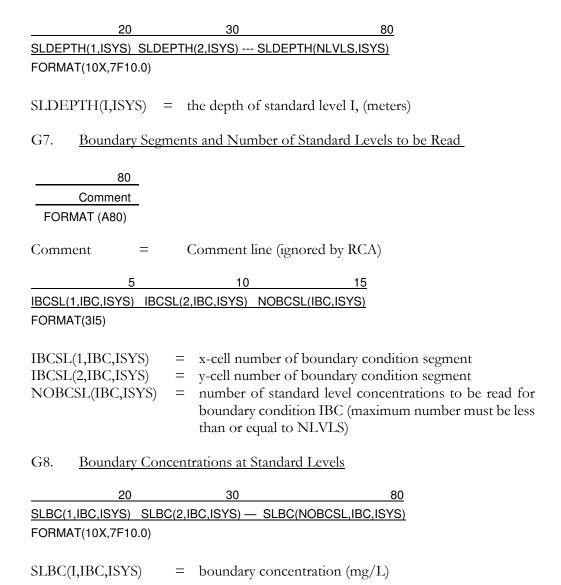
specify boundary concentration information for system ISYS

### G6. Standard Level Depths

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)





After reading in the boundary concentrations at the standard levels RCA will perform a linear interpolation of the input data onto the sigma level grid and produce a set of boundary segment numbers (IX,IY and IZ) and concentrations similiar to the input required for IBCOPT = 2.

After input types G2 through G8 are read for each system, then the time of the next set of boundary concentrations, NXBCT, will be required; followed by the next set of boundary concentrations specified at standard levels (input type G8); it is not necessary to repeat input types G2 through G7.

Table 5 presents an example of a boundary condition input file using time-variable sigma level input (IBCOPT = 2), while Table 6 presents an example of a boundary condition input file using time-invariant or constant standard level input.



#### TABLE 5. EXAMPLE OF TIME-VARIABLE SIGMA-LEVEL BOUNDARY CONDITIONS - BCFILNA PWLOPT base values - no additions to PO4, NH3, Si for algal biomass NXBCTSECS TWARPBC time JAN 1 ,81 NOBC no. of boundary condition segments С SCALBC scale factor LOCATIONS OF BOUNDARY SEGMENTS bc segs 2 1 1 2 1 2 1salinity .3070E+02 .3070E+02 NOBC no. of boundary condition segments С SCALBO Scale factor LOCATIONS OF BOUNDARY SEGMENTS bc segs 2 1 1 2 1 2 2 2 2Wint Phy .1750E+00 .1750E+00 NOBC no. of boundary condition segments С SCALBO 1.0 scale factor C LOCATIONS OF BOUNDARY SEGMENTS bc segs 2 1 1 2 1 2 3Summ Phy .5250E-01 .5250E-01 C NOBC no. of boundary condition segments С SCALBO LOCATIONS OF BOUNDARY SEGMENTS segs 2 1 1 2 1 2 scale factor 2 1 1 2 1 2 .1000E-05 .1000E-05 4 RPOP NOBC no. of boundary condition segments 0 scale factor LOCATIONS OF BOUNDARY SEGMENTS bc segs 2 1 1 2 1 2 .1000E-05 .1000E-05 NOBC no. of boundary condition segments SCALBO 0 scale factor LOCATIONS OF BOUNDARY SEGMENTS bc segs 2 1 1 2 1 2 6 RDOP .1000E-02 .1000E-02 NOBC no. of boundary condition segments scale factor LOCATIONS OF BOUNDARY SEGMENTS bc segs 7 LDOP NOBC 2 1 1 2 1 2 .4000E-02 .4000E-02 no. of boundary condition segments С SCALBC ) scale factor LOCATIONS OF BOUNDARY SEGMENTS bc segs 2 1 1 2 1 2 8Tot PO4 .3844E-01 .3844E-01 no. of boundary condition segments SCALBC С scale factor LOCATIONS OF BOUNDARY SEGMENTS bc segs 9 RPON NOBC 2 1 1 2 1 2 .1000E-05 .1000E-05 C no. of boundary condition segments 2 SCALBC С C LOCATIONS OF BOUNDARY SEGMENTS bc segs 2 1 1 2 1 2 10 LPON .1000E-05 .1000E-05 C NOBC no. of boundary condition segments С C LOCATIONS OF BOUNDARY SEGMENTS bc segs 2 1 1 2 1 2 1 1 RDON .1000E-02 .1000E-02 11 RDON C NO NOBC no. of boundary condition segments C SCALBC 1.0 0 scale factor LOCATIONS OF BOUNDARY SEGMENTS bc segs 12 LDON C NOBC 2 1 1 2 1 2 .8000E-02 .8000E-02 NOBC no. of boundary condition segments scale factor LOCATIONS OF BOUNDARY SEGMENTS 2 1 1 2 1 2 bc segs 2 1 1 2 1 2 13 Tot NH4 .7062E-01 .7062E-01



```
TABLE 5. EXAMPLE OF TIME-VARIABLE SIGMA-LEVEL BOUNDARY CONDITIONS - BCFILNA (Cont.)
                                                             no. of boundary condition segments
 С
       SCALBO
                 Scale factor LOCATIONS OF BOUNDARY SEGMENTS
bc segs
14 NO23
C
       segs 2 1 1 2 1 2
NO23 .1050E+00 .1050E+00
NOBC
                                                            no. of boundary condition segments
 С
      SCALBO
           1.0 scale factor
LOCATIONS OF BOUNDARY SEGMENTS
 bc segs 2 1 1 2 1 2 1 5 BioG Si .1000E-05 .1000E-05 C NOBC
                                                            no. of boundary condition segments
 С
       SCALBO
DC Segs 2 1 1 2 1 2 1 2 16 TOT SI .2413E+00 .2413E+00 C NOBC
                                                            no. of boundary condition segments
                0 scale factor
LOCATIONS OF BOUNDARY SEGMENTS
  bc segs
                   2 1 1 2 1 2
.1000E-05 .1000E-05
 17 RPOC
C N
        NOBC
                                                            no. of boundary condition segments
C LOCATIONS OF BOUNDARY SEGMENTS bc segs 2 1 1 2 1 2 18 LPOC .1000E-05 .1000E-05 C NOBC
                                                             no. of boundary condition segments
                 scale factor LOCATIONS OF BOUNDARY SEGMENTS
        1.0
 bc segs
19 RDOC
C NOBC
                   2 1 1 2 1 2
.1000E-05 .1000E-05
                                                            no. of boundary condition segments
 С
       SCALBC
                 scale factor LOCATIONS OF BOUNDARY SEGMENTS
       1.0
 С
 bc segs
20 LDOC
C NOBC
                  2 1 1 2 1 2
.1000E-05 .1000E-05
                                                            no. of boundary condition segments
                                                          scale factor
             LOCATIONS OF BOUNDARY SEGMENTS
bc segs
21 REDOC
C NOBC
                  2 1 1 2 1 2
.1000E-05 .1000E-05
                                                            no. of boundary condition segments
 С
       SCALBO
                 scale factor LOCATIONS OF BOUNDARY SEGMENTS
 bc segs
22 EXDOC
C NOBC
                   2 1 1 2 1 2
.1000E-05 .1000E-05
                                                            no. of boundary condition segments
 С
       SCALBO
1.0 scale factor
C LOCATIONS OF BOUNDARY SEGMENTS
bc segs 2 1 1 2 1 2
23 AQ SOD .0000E+00 .0000E+00
C NOBC
                                                            no. of boundary condition segments
                U Scale factor LOCATIONS OF BOUNDARY SEGMENTS 2 1 1 2 1 2 1 2 .1141E+02 .31
  bc segs
DC Segs 2 1 1 2 1 2
24 DO .1141B+02 .1141B+02
.1141B+02 .1141B+02
.2wint phy .2350E+00 .2350E+00
.3summ phy .4050E-01 .4050E-01
.4rpop .1000E-05 .1000E-05
.6rdop .1000E-02 .1000E-05
.7ldop .4000E-02 .4000E-02
.7ldop .4000E-02 .4000E-02
.7ldop .1000E-05 .1000E-05
.7ldop .1000E-05 .1000E-05
.7ldop .1000E-05 .1000E-05
.7ldop .1000E-05 .1000E-05
.1 rdon .1000E-05 .1000E-05
.1 rdon .8000E-02 .8000E-02
.12 ldon .8000E-02 .8000E-02
.13 nh3 tot .7545E-01 .7545E-01
.14 no23 .1060E+00 .1060E+00
.15 bio si .1000E-05 .1000E-05
.16 tot si .2919E+00 .2919E+00
.7 rpoc .1000E-05 .1000E-05
 24 DO
                                                    FEB 1 81
```



```
TABLE 5. EXAMPLE OF TIME-VARIABLE SIGMA-LEVEL BOUNDARY CONDITIONS - BCFILNA (Cont.)
lpoc
rdoc
             .1000E-05 .1000E-05 .1000E-05
                                       81
     This portion of input file, covering the period from April through Oct is not being shown
 NOV 1
                                         81
                                DEC 1
                                         81
                               time JAN 1, 82 - end of simulation
```



## TABLE 6. EXAMPLE OF TIME-INVARIANT STANDARD LEVEL BOUNDARY CONDITION INPUT-BCFILNA

```
IBCLOPT
                                                      NOBC
     14
C SCALBC - scale factor
                              1.
NLVLS - No of Std Lvl Depths
C NLVLS - No of Std Lv1 Depths
4
C Standard Level Depths
SLDPTHS 0.00 20.00 60.00 110.00
C BC Locations/# of Stardard Level Data to read (IX, IY, NSTLVLS)
Salinity 19 6 4 19 7 4 19 8 4 19 9 4 19 10 4 19 11 4 19 12 4
19 13 4 19 14 4 19 15 4 19 16 4 19 17 4 19 18 4 19 19 4
C Salinity boundary condition data for each standard level
19, 6 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 7 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 8 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 9 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 10 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 10 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 11 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 12 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 13 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 14 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 15 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 16 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 17 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 18 0.3240E+020.3240E+020.3250E+020.3250E+02
19, 19 0.3240E+020.3240E+020.3250E+020.3250E+02
                                      NOBC
14
SCALBC - scale factor
                                             NLVLS - No of Std Lvl Depths
 C Standard Level Depths
SLDPTHS 0.00 20.00 60.00 110.00
C BC Locations/# of Stardard Level Data to read (IX,IY,NSTLVLS)
Phytol 19 6 4 19 7 4 19 8 4 19 9 4 19 10 4 19 11 4 19 12 4
19 13 4 19 14 4 19 15 4 19 16 4 19 17 4 19 18 4 19 19 6
C Phytoplankton - Algal Group 1 boundary condition data for each standard level PHYT1 0.2000E-010.1500E-010.1000E-010.5000E-02
                                                                                            0.2000E-010.1500E-010.1000E-010.5000E-02

0.2000E-010.1500E-010.1000E-010.5000E-02

0.2000E-010.1500E-010.1000E-010.5000E-02

0.2000E-010.1500E-010.1000E-010.5000E-02

0.2000E-010.1500E-010.1000E-010.5000E-02

0.2000E-010.1500E-010.1000E-010.5000E-02
                                                      NOBC
                                      14
SCALBC - scale factor
     С
                                           NLVLS - No of Std Lvl Depths
     С
C NLVLS - No of Std Lvl Depths
4

C Standard Level Depths
SLDPTHS 0.00 20.00 60.00 110.00

C BC Locations/# of Standard Level Data to read (IX,IY,NSTLVLS)
Phyto2 19 6 4 19 7 4 19 8 4 19 9 4 19 10 4 19 11 4 19 12 4
19 13 4 19 14 4 19 15 4 19 16 4 19 17 4 19 18 4 19 19

C Phytoplankton - Algal Group 2 boundary condition data for each standard level
PHYT2 0.5000E-020.5000E-020.2000E-020
0.5000E-020.5000E-020.2000E-020.2000E-02
0.5000E-020.5000E-020.2000E-020.0000E-02
0.5000E-020.5000E-020.2000E-020.2000E-02
0.5000E-020.5000E-020.2000E-020.000E-02
0.5000E-020.5000E-020.2000E-020.2000E-02
                                                                                                0.5000E-020.5000E-020.2000E-020.2000E-02
0.5000E-020.5000E-020.2000E-020.2000E-02
                                                                                                                rest of boundary input not displayed
                                                                                                              //////////
```



## GROUP H: POINT SOURCE LOADS (PSFILNA)

Inputs required for this group include:

- 1. point source loads input option
- 2. index table of point source loads
- 3. number of point source loads
- 4. scale factor for point source loads
- 5. actual point source loads

## H1. Point Source Loads Input Option

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

FORMAT (2I10)

**IPSPWLOPT** 

IPSOPT = input option

= 1, all point source loads are constant in time

= 2, time-variable point source loads will be used option to select step-function or piecewise linear interpolation

of time-variable point source loadings.

= 0, step-function interpolation will be used

= 1, piecewise linear interpolation will be used

The remaining point source loads inputs are dependent upon the IPSOPT input option chosen. Data inputs for option 1 (constant loads) will be presented first, followed by data inputs associated with option 2 (time-variable).

#### H2. <u>Index Table of Point Source Loads</u>

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

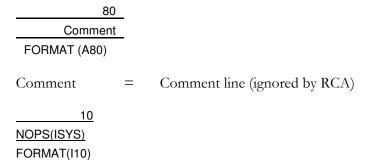


5		10	15		65_		
IPS(1,I,ISYS)	IPS(2	,I,ISY)	IPS(3,I,ISYS)	LOCATION	N		
FORMAT (3I5,A5	(0)						
IPS(1,I,ISYS)	=	throug model	gh the number	of point	mbered consecutively from 1 source loads included in the		
IPS(2,I,ISYS)	=	the x-	cell number of	the point			
IPS(3,I,ISYS) LOCATION	=	the y-cell number of the point source load. a 50-character alpha-numeric description of the point source load locations, ex. Blue Plains WWTP					
16		2	22	70_			
ZFRACPS(1,I)	ZFRA	ACPS(2	I) ZFRACE	PS(NZ,I)			
FORMAT (10X,10	0F6.3)						
ZFRACPS(1,I) : ZFRACPS(NZ,I)	=	If a us water ZFRA put a l	gh NZ (note: froser wished to column and if CPS(10,I) would and in the bott	ractions shifted stribute in NZ=10, all deach become two certains.	ischarged to layer 1,2,, nould sum up to 1.0) a load equally throughout the then ZFRACPS(1,I) through e set to 0.1. If a user wished to ells only (and again if NZ=10), ZFRACPS(8,I) = 0.0, and		
			ZFRACPS(1,1) .CPS(9,I) = ZF		* * *		

## Constant or Time-Invariant Loads (IPSOPT = 1)

Data associated with Data Types H3, H4 and H5 will be read NOSYS times; once for each system in the model.

## H3. Number of Point Source Loads





NOPS(ISYS) = the number of point source loads for system ISYS

(Note: If there are no point source loads to be specified for a system (NOPS = 0), then no input is required for H4 or H5; just continue with next H3.

#### H4. Point Source Load Scale Factor

Comment FORMAT (A80)

Comment ine (ignored by RCA)

SCALPS(ISYS) FORMAT(F10.0)

SCALPS(ISYS) = scale factor system ISYS

Normally SCALPS(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in point source inputs, SCALPS(ISYS) would then be set equal to 0.75.

#### H5. Point Source Loading Segments and Point Source Loads

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 15 70 75

BPS(1,ISYS) IPS(1,ISYS) . . . BPS(NOPS,ISYS) IPS(NOPS,ISYS)

FORMAT(5(F10.0,I5)

BPS(I,ISYS) = point source load (kg/day)

IPS(I,ISYS) = index number of the point source load



<u>Time-Variable Conditions (IPSOPT = 2)</u>

#### H3. <u>Time of Point Source Loading Specifications</u>

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

20 30

NXPSTSECS TWARPPS

FORMAT (10X, I10,6X,A4)

NXPSTSECS = time in seconds (or units specified by TWARPPS

TWARPPS = units to be used for NXPSTSECS

SECS or secs,MINS or mins,HRS or hrs,DAYS or days.

Data associated with Data Types H4 through H7 will be read NOSYS times; once for each system in the model.

#### H4. Number of Point Source Loads

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

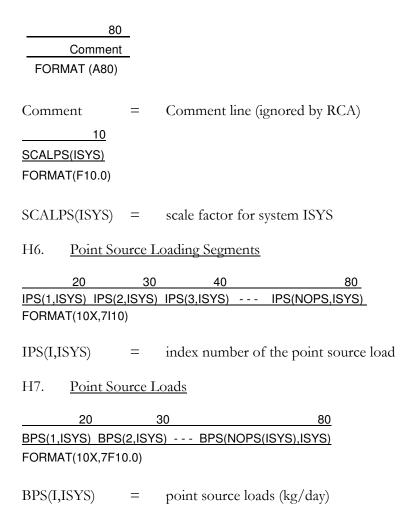
NOPS(ISYS) FORMAT(I10)

NOPS(ISYS) = the number of point source loads for system ISYS

(Note: if NOPS equal zero, then skip H5, H6 and H7 and continue with next H4 input.)

#### H5. Point Source Loads Scale Factor





After input types H4 through H7 are repeated for each system, then the time of the next set of point source loads, NXPST, will be required; followed by the next set of point source loads (input type H7); it is not necessary to repeat input types H4, H5 and H6. If NOPS (ISYS) = 0 for system ISYS then no input type H7 is required either.

Table 7 presents an example input file for constant loading point source inputs. The user is referred back to Table 6 under GROUP G for an example of what a time-variable point source input file would look like.



T.	ABLE 7. EXAMPLE	OF TIME-INVARIANT OR	CONSTANT POINT SOL	JRCE INPUT - PSFILNA
С	NO IX IY Loc	ation / Vertical Distri	bution Fractions (I	index of Point Source Loads)
F	1 5 16 Blu ractions 0.25 0.25	e Plains WWTP 0.25 0.25 0. 0.	0. 0. 0. 0.	ndex of Point Source Loads)
	2 16 4 Dee			
	3 16 5 Nut	Island WWTP	0. 0. 0. 0.	
	4 11 28 Tal	lman Island		
	5 3 17 Rye	0.1 0.1 0.1 0.1 0 Brook WWTP		
С	-99 End	0. 0. 0. 0. of Point Source Loading nt source loads for sys	g Table Index	
С	0	of loads for system 2		
С	SCALPS(2) - scale	factor		
С	Load IPS	Load IPS Load IPS 78. 2 6.3 4	Load IPS I	oad IPS
С	NOPS(3) - number	of loads for system 3	23. 4	43. 3
С	SCALPS(3) - scale	factor		
С		Load IPS Load IPS 75. 2 6.0 4	Load IPS I	oad IPS
С	NOPS(4) - number	of loads for system 4	22. 4	40. 5
С	SCALPS(4) - scale	factor		
С	1.0 Load IPS	Load IPS Load IPS 10. 2 0.7 4	Load IPS I	oad IPS
С	NOPS(5) - number	of loads for system 5	2. 4	4. 5
С	SCALPS(5) - scale	factor		
С	1.0 Load IPS	Load IPS Load IPS 10. 2 2. 4	Load IPS I	oad IPS
С	NOPS(6) - number	of loads for system 6	4. 5	
С	SCALPS(6) - scale	factor		
С	1.0 Load IPS	Load IPS Load IPS 1010. 2 250. 4	Load IPS I	oad IPS
С	NOPS(7) - number	of loads for system 7	825. 4 4	60. 5
С	SCALPS(7) - scale	factor		
С	Load IPS	Load IPS Load IPS 110. 2 10.7 4	Load IPS I	oad IPS 74. 5
С		of loads for system 8	22.	
С	SCALPS(8) - scale	factor		
С	Load IPS	Load IPS Load IPS 310. 2 17. 4	Load IPS I	oad IPS 66. 5
С	NOPS(9) - number	of loads for system 9	J2. 4	00. 3
С	SCALPS(9) - scale	factor		
С	1.0 Load IPS	Load IPS Load IPS 20. 2 8. 4	Load IPS I	oad IPS
С	NOPS(10) - number	of loads for system 10	33. 4	24. 3
С	5 SCALPS(10) - scal 1.0			
С	Load IPS	Load IPS Load IPS 510. 2 16. 4	Load IPS I 89. 4	load IPS 27. 5



# GROUP I: NONPOINT SOURCE LOADS (NPSFILNA)

Inputs required for this group include:

- 1. nonpoint source loads input option
- 2. index table of nonpoint source loads
- 3. number of nonpoint source loads
- 4. scale factor for nonpoint source loads
- 5. actual nonpoint source loads

#### I1. Nonpoint Source Loads Input Option

Comment FORMAT (A80)

Comment | = Comment line (ignored by RCA)

10 20

INPSOPT INPSPWLOPT

FORMAT (2012)

FORMAT (2I10)

INPSPWLOPT =

INPSOPT = input option

= 1, all nonpoint source loads are constant in time

= 2, time-variable nonpoint source loads will be used option to select step-function or piecewise linear interpolation

of time variable nonpoint source loadings

= 0, step function interpolation will be used,

= 1, piecewise linear interpolation will be used

The remaining nonpoint source loading inputs are dependent upon the INPSOPT input option chosen. Data inputs for option 1 (constant loads) will be presented first, followed by data inputs associated with option 2 (time-variable).

#### I2. <u>Index Table of Nonpoint Source Loads</u>

Comment FORMAT (A80)

Comment ine (ignored by RCA)



5	10	15	65	<u>.                                    </u>
INPS(1,I,ISYS)	INPS(2,I,ISY)	INPS(3,I,ISYS)	LOCATION	
FORMAT (315,A	.50)			
INPS(1,I,ISYS)	through model	`	nonpoint sour	d consecutively from 1 rce loads included in the
INPS(2,I,ISYS)		ell number of the	1	urce load
INPS(3,I,ISYS)		ell number of the		
LOCATION		haracter alpha-nu load locations, ex		iption of the nonpoint CSO
16	6 2	22	70	
ZFRACNPS(1,I)	) ZFRACNPS	S(2,I) ZFRAC	NPS(NZ,I)	
FORMAT (10X,	10F6.3)		· <del></del>	

ZFRACNPS(1,I) = fraction of point source load discharged to layer 1,2, ..., through NZ (note: fractions should sum up to 1.0)

ZFRACPS(NZ,I) If a user v

If a user wished to distribute a load equally throughout the water column and if NZ=10, then ZFRACNPS(1,I) through ZFRACNPS(10,I) would each be set to 0.1. If a user wished to put a load in the bottom two cells only (and again if NZ=10), then ZFRACNPS(1,I) through ZFRACNPS(8,I) = 0.0, and ZFRACNPS(9,I) = ZFRACNPS(10,I) = 0.5

#### Constant or Time-Invariant Loads (INPSOPT = 1)

Data associated with Data Types I3, I4 and I5 will be read NOSYS times; once for each system in the model.

#### I3. Number of Nonpoint Source Loads

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)



NONPS(ISYS) FORMAT(I10)

NONPS(ISYS) = the number of nonpoint source loads for system ISYS

(Note: If there are no non-point source loads to be specified for a system (NONPS = 0), then no input is required for I4 or I5; just continue with next I3.

#### I4. Nonpoint Source Load Scale Factor

Comment FORMAT (A80)

Comment | Comment line (ignored by RCA)

\_\_\_\_\_10 SCALNPS(ISYS)

FORMAT(F10.0)

SCALNPS(ISYS) = scale factor for system ISYS

Normally SCALNPS(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in nonpoint source inputs, SCALNPS(ISYS) would then be set equal to 0.75.

#### I5. Nonpoint Source Loading Segments and Nonpoint Source Loads

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 15 70 75

BNPS(1,ISYS) INPS(1,ISYS) --- BNPS(NONPS,ISYS) INPS(NONPS,ISYS) FORMAT(5(F10.0,I5)

BNPS(I,ISYS) = nonpoint source load (kg/day)

INPS(I,ISYS) = index number of the nonpoint source load



<u>Time-Variable Conditions (INPSOPT = 2)</u>

#### 13. <u>Time of Nonpoint Source Loading Specifications</u>

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

20 30

NXNPSTSECS TWARPNPS

FORMAT (10X, I10,6X,A4)

NXNPSTSECS = time in seconds (or units specified by TWARPNPS)

TWARPNPS = units to be used for NXNPSTSECS

= SECS or secs,= MINS or mins,= HRS or hrs,= DAYS or days.

Data associated with Data Types I4 through I7 will be read NOSYS times; once for each system in the model.

#### I4. Number of Nonpoint Source Loads

Comment FORMAT (A80)

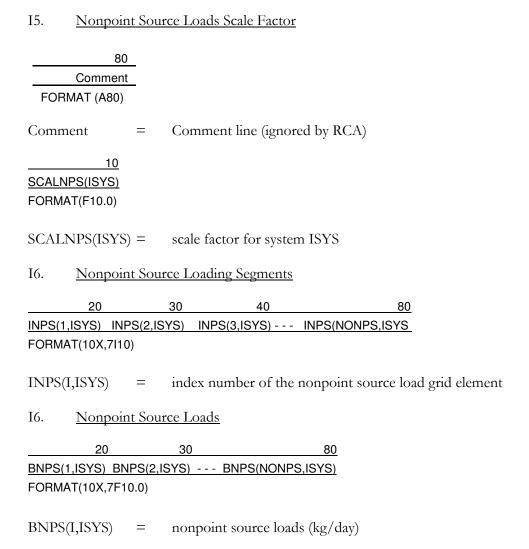
Comment = Comment line (ignored by RCA)

NONPS(ISYS) FORMAT(I10)

NONPS(ISYS) = the number of nonpoint source loads for system ISYS

(Note: if NONPS equal zero, then skip I5, I6 and I7 and continue with next I4 input.)





After input types I4 through I7 are repeated for each system, then the time of the next set of nonpoint source loads, NXNPST, will be required; followed by the next set of nonpoint source loads (input type I7); it is not necessary to repeat input types I4, I5 and I6. If NONPS (ISYS) = 0 for system ISYS then no input type I7 is required either.

The user is referred back to Tables 6 and 7 for examples of what time-variable and constant input files would look like.



## GROUP J: FALL-LINE LOADS (FLFILNA)

Inputs required for this group include:

- 1. fall-line loads input option
- 2. index table of fall-line loads
- 3. number of fall-line loads
- 4. scale factor for fall-line loads
- 5. actual fall-line loads

#### J1. Fall-line Loads Input Option

80
Comment
FORMAT (A80)

Comment ine (ignored by RCA)

10 IFLOPT IFLPWLOPT FORMAT(2I10)

IFLOPT = input option

= 1, all fall-line loads are constant in time

= 2, time-variable fall-line loads will be used

IFLPWLOPT = option to select step-function or piecewise linear interpolation

of time-variable fall-line source loadings.

= 0, step function interpolation will be used,

= 1, piecewise linear interpolation will be used.

The remaining fall-line loading inputs are dependent upon the IFLOPT input option chosen. Data inputs for option 1 (constant loads) will be presented first, followed by data inputs associated with option 2 (time-variable).

#### J2. <u>Index Table of Fall-Line Loads</u>

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

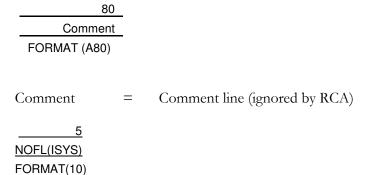


5		10	15	65	
IFL(1,I,ISYS)	IFL(2,I	,ISY)	IFL(3,I,ISYS)	LOCATION	
FORMAT (315,A	<b>\</b> 50)				
IFL(1,I,ISYS)	=	throu	`	of fall-line lo	ered consecutively from 1 pads included in the model
IFL(2,I,ISYS)	=	the x-	-cell number of	f the fall-line l	load
IFL(3,I,ISYS)	=	the y-	cell number of	the fall-line l	oad.
LOCATION	=	a 50-c	character alpha	-numeric des	cription of the fall-line load
		locati	ons, ex. Brancl	n Brook Inflo	W
16			22	70_	
ZFRACFL(1,I)	ZFI	RACFL	(2,I) ZFRA	CFL(NZ,I)	
FORMAT (10X,					
	, ,				
ZFRACFL(1,I)		=	fraction of f	all-line load d	lischarged to layer 1,2,,
:					ons should sum up to 1.0)
ZFRACFL(NZ,	I)		throughout ZFRACFL( be set to 0.7 bottom two ZFRACFL(	the water co 1,I) through 7 1. If a user vo cells only (a 1,I) through	distribute a load equally blumn and if NZ=10, then ZFRACFL(10,I) would each wished to put a load in the and again if NZ=10), then ZFRACFL(8,I) = 0.0, and CFL(10,I) = 0.5

#### Constant or Time-Invariant Loads (IFLOPT = 1)

Data associated with Data Types J3, J4 and J5 will be read NOSYS times; once for each system in the model.

#### J3. Number of Fall-line Loads





NOFL(ISYS) = the number of fall-line loads for system ISYS

(Note: If there are no fall-line loads to be specified for a system (NOFL = 0), then no input is required for J4 or J5; just continue with next J3.)

#### J4. <u>Fall-line Load Scale Factor</u>

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

 $\frac{10}{\text{SCALFL(ISYS)}}$ FORMAT(F10.0)

SCALFL(ISYS) = scale factor for system ISYS

Normally SCALFL(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in fall-line inputs, SCALFL(ISYS) would then be set equal to 0.75.

#### J5. Fall-line Loading Segments and Fall-line Loads

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 15 70 75

BFL(1,ISYS) IFL(1,ISYS) BFL(NOFL,ISYS) IFL(NOFL,ISYS)

FORMAT(5(F10.0,I5))

BFL(I,ISYS) = fall-line load (kg/day)

IFL(I,ISYS) = index number of the fall-line load



<u>Time-Variable Conditions (IFLOPT = 2)</u>

#### J3. <u>Time of Fall-line Loading Specifications</u>

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

NXFLTSECS = time in seconds (or units specified by TWARPFL)

TWARPFL = units to be used for NXFLTSECS

= SECS or secs, = MINS or mins, = HRS or hrs, = DAYS or days.

Data associated with Data Types J4 through J7 will be read NOSYS times; once for each system in the model.

#### J4. Number of Fall-line Loads

Comment FORMAT (A80)

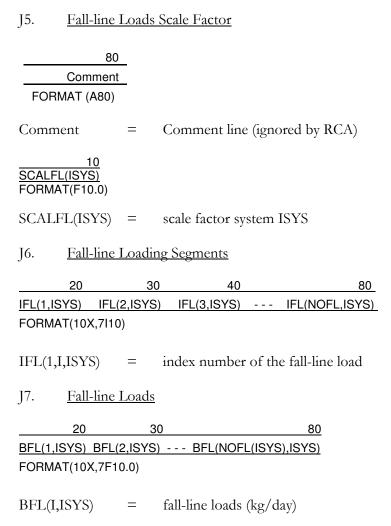
Comment = Comment line (ignored by RCA)

5 NOFL(ISYS) FORMAT(10)

NOFL(ISYS) = the number of fall-line loads for system ISYS

(Note: if NOFL equal zero, then skip J5, J6 and J7 and continue with next J4 input.)





After input types J4 through J7 are repeated for each system, then the time of the next set of fall-line loads, NXFLT, will be required; followed by the next set of fall-line loads (input type J7); it is not necessary to repeat input types J4, J5 and J6. If NOFL (ISYS) = 0 for system ISYS then no input type J7 is required either.

The user is referred back to Tables 6 and 7 for examples of what time-variable and constant input files would look like.



# GROUP K: ATMOSPHERIC LOADS (ATMFILNA)

Inputs required for this group include:

- 1. atmospheric loads input option
- 2. number of atmospheric loads
- 3. scale factor for atmospheric loads
- 4. actual atmospheric loads

#### K1. Atmospheric Loads Input Option

Comment FORMAT (A80)

Comment | = Comment line (ignored by RCA)

10 20
IATMOPT IATMPWLOPT
FORMAT (2I10)

IATMOPT = input option

= 1, all atmospheric loads are constant in time

= 2, time-variable atmospheric loads will be used

IATMPWLOPT = option to select step-function or piecewise linear interpolation

of time-variable atmospheric loadings.

= 0, step-function interpolation will be used,

= 1, piecewise linear interpolation will be used.

The remaining atmospheric loading inputs are dependent upon the IATMOPT input option chosen. Data inputs for option 1 (constant loads) will be presented first, followed by data inputs associated with option 2 (time-variable).

#### Constant or Time-Invariant Loads (IATMOPT = 1)

Data associated with Data Types K2, K3 and K4 will be read NOSYS times; once for each system in the model.

#### K2. Number of Atmospheric Loads

Comment FORMAT (A80)



Comment ine (ignored by RCA)

NOATM(ISYS)

FORMAT(I10)

NOATM(ISYS) = the number of atmospheric loads for system ISYS

= 0, no atmospheric loading for system ISYS

= 1, spatially-constant atmospheric loadings to water surface

= 2, spatially-variable atmospheric loadings to water surface

(Note: If there are no atmospheric inputs to be specified for a system (NOATM = 0), then no input is required for K3 or K4; just continue with next K2.

#### K3. Atmospheric Load Scale Factor

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

1

SCALATM(ISYS)

FORMAT(F10.0)

SCALATM(ISYS) = scale factor for system ISYS

Normally SCALATM(ISYS) would be set equal to 1.0, however, if the user wished to perform a sensitivity run to a 25 percent reduction in atmospheric inputs, SCALATM(ISYS) would then be set equal to 0.75.

Spatially Constant Atmospheric Loads (NOATM (ISYS=1)

#### K4. Atmospheric Loading Rate

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)



20 BATM(ISYS) FORMAT(10X,F10.0)

BATM(ISYS) = atmospheric loading rate  $(kg/m^2-day)$ 

RCA will take the areal atmospheric loading rate for system ISYS and apply this loading rate to each water segment in the model by multiplying the wetted surface area of the segment by the areal loading rate to compute the total kg/day loading to the water segment.

<u>Spatially-Variable Atmospheric Loads (NOATM = 2)</u>

#### K4. <u>Atmospheric Loading Rates</u>

BATM(IX,IY,ISYS) = atmospheric loading rate (kg/m²-day) for segment or grid cell (IX,IY) for system ISYS

<u>Time-Variable Conditions (IATMOPT = 2)</u>

#### K2. <u>Time of Atmospheric Loading Specifications</u>

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

NXATMTSECS = time in seconds (or units specified by TWARPATM

TWARPATM = units to be used for NXATMTSECS

= SECS or secs,



= MINS or mins,= HRS or hrs,= DAYS or days.

Data associated with Data Types K3, K4 and K5 will be read NOSYS times; once for each system in the model.

#### K3. Number of Atmospheric Loads

Comment FORMAT (A80)

Comment ine (ignored by RCA)

5 NOATM(ISYS) FORMAT(10)

NOATM(ISYS) = the number of atmospheric loads for system ISYS

= 0, for no atmospheric loading for system ISYS

= 1, spatially-constant atmospheric loading to water surface

= 2, spatially-variable atmospheric loadings to water surface (Note: if NOATM equal zero, then skip K4 and K5 and continue with next K3 input.)

#### K4. <u>Atmospheric Loads Scale Factor</u>

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 SCALATM(ISYS) FORMAT(F10.0)

SCALATM(ISYS) = scale factor for system ISYS



Spatially-Constant Atmospheric Loading (NOATM(ISYS) = 1)

K5. Atmospheric Loading Rate

Comment FORMAT (A80)

Comment ine (ignored by RCA)

<u>20</u> BATM(ISYS) FORMAT(10X,F10.0)

BATM(ISYS) = atmospheric loading rate (kg/m2-day)

Spatially-Variable Atmospheric Loads (NOATM(ISYS) = 2)

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

K5. Atmospheric Loading Rates

<u>20</u> <u>30</u> <u>80</u> <u>BATM(1,NY,ISYS)</u> <u>BATM(2,NY,ISYS) - - - BATM(NX,NY,ISYS)</u> <u>FORMAT(10X,7F10.0)</u>

BATM(IX,IY,ISYS) = atmospheric loading rate for segment or grid cell (IX,IY) for system ISYS

After input types K3 through K5 are repeated for each system, then the time of the next set of atmospheric loads, NXATMT, will be required; followed by the next set of atmospheric loads (input type K5); it is not necessary to repeat input types K3 and K4. If NOATM (ISYS) = 0 for a system then no input type K5 is required either.

RCA will take the areal atmospheric loading rate for system ISYS and apply it to each water segment in the model by and multiplying the wetted surface area of the receiving water segment by the loading rate to compute the total kg/day loading to the segment.



Tables 8 and 9 provide example input files for constant and time-variable inputs.



### TABLE 8. EXAMPLE OF TIME-INVARIANT OR CONSTANT POINT SOURCE INPUT - PSFILNA C IATMOPT

```
C NOATM(1)
            no salinity loads
C NOATM(2) no phytoplankton loads
C NOATM(3)
            no phytoplankton loads
C NOATM(4)
            no RPOP loads
C NOATM(5) no LPOP loads
C NOATM(6)
            no RDOP loads
C NOATM(7) no LDOP loads
C NOATM(8) DPO4 load
C SCALATM
C PO4 load (kg/m2-day) == 0.011 mg P/L * 47 inches rainfall/yr 0.3600E-07
C NOATM(9) no RPON loads
C NOATM(10) no LPON loads
C NOATM(11) no RDON loads
C NOATM(12) no LDON loads
C NOATM(13) NH4 loads
C SCALATM
1.0
C NH4 load (kg/m2-day) == 0.15 mg N/L * 47 in/yr = 0.15 g N/m3 * 1.194 m/yr * yr/365 day *
C NH4 10
kg/1000 g
0.4907E-06
C NOATM(14) NO3 loads
C SCALATM
      1.0
C NO3 load (kg/m2-day) == 0.43 \text{ mg N/L} * 47 \text{ in/yr}
1.4066E-06
C NOATM(15) no BSi loads
C NOATM(16) no DSI loads
  loads
C NOATM(17) no RPOC loads
C NOATM(18) no LPOC loads
C NOATM(19) no RDOC loads
C NOATM(20) no LDOC loads
C NOATM(21) no ReDOC loads
C NOATM(22) no ExDOC loads
C NOATM(23) no O2eq loads
C NOATM(24) no DO loads
```



#### TABLE 9. EXAMPLE OF TIME-VARIABLE ATMOSPHERIC INPUT - ATMFILNA TABLE IATMOPT IATMPWLOPT NXATMTSECS TWARPATM C NOATM(1) no salinity load NOATM(2) no phytoplankton load NOATM(3) no phytoplankton load С NOATM(4) no RPOP load С NOATM(5) no LPOP load NOATM(6) no RDOP load С NOATM(7) no LDOP load С NOATM(8) DPO4 load assumes 0.011 mg P/L in rainfall and the value specified by BATM is monthly-averaged rainfall in inches/day SCALATM 2.794E-06 PO4 load following value is total rainfall in January (3.1 inches) / 31 days 0.100 NOATM(9) no RPON load C NOATM(10) no LPON load C NOATM(11) no RDON load no LDON load C NOATM(13) NH4 load assumes 0.15 mg N/L in rainfall and the value specified by BATM is monthly-averaged rainfall in inches/day following value is total rainfall in January (3.1 inches) / 31 days SCALATM 3.810E-05 C NH4 load 0.100 NO3 load C NOATM(14) C SCALATM assumes 0.43 mg $\rm N/L$ in rainfall and the value specified by BATM is monthly-averaged rainfall in inches/day 1.092E-04 following value is total rainfall in January (3.1 inches) / 31 days 0.100 C NO3 load C NOATM(15) no BSi load C NOATM(16) no DSI load C NOATM(17) no RPOC load C NOATM(18) no LPOC load C NOATM(19) no RDOC load C NOATM(20) no LDOC load C NOATM(21) no ReDOC load C NOATM(22) no ExDOC load C NOATM(23) no O2eq load C NOATM(24) no DO load TIME 2.18 inches / 28 days 2.18 inches / 28 days 2.18 inches / 28 days 0.07786 PO4 NH4 0.07786 NO3 0.07786 TIME 59 3.28 inches / 31 days 3.28 inches / 31 days 3.28 inches / 31 days PO4 0.10581 NH4 0.10581 0.10581 NO3 TIME 0.08500 2.55 inches / 30 days 2.55 inches / 30 days 2.55 inches / 30 days PO4 NH4 0.08500



NO3

TIME

0.08500

120 0.08903

2.76 inches / 31 days

TABLE 9. EXAMPLE OF TIME-VARIABLE ATMOSPHERIC INPUT - ATMFILNA TABLE (Cont.)

NH4	0.08903	2 76		,	2.1	-1
			inches			
NO3	0.08903	2.76	inches	/	31	aays
TIME	151					
PO4	0.01060	3.18				
NH4	0.01060	3.18				days
NO3	0.01060	3.18	inches	/	30	days
TIME	181					
PO4	0.04871	1.51				
NH4	0.04871	1.51	inches	/	31	days
NO3	0.04871	1.51	inches	/	31	days
TIME	212					
PO4	0.03581	1.11	inches	/	31	days
NH4	0.03581	1.11	inches	/	31	days
NO3	0.03581	1.11	inches			
TIME	243					_
PO4	0.13500	4.05	inches	/	30	days
NH4	0.13500	4.05	inches	/		days
NO3	0.13500	4.05	inches	/		davs
TIME	273					-
PO4	0.06484	2.01	inches	/	31	davs
NH4	0.06484	2.01				
NO3	0.06484	2.01				
TIME	304					2
PO4	0.08266	2.48	inches	/	30	davs
NH4	0.08266	2.48				
NO3	0.08266	2.48				
TIME	334			′		51017
PO4	0.05677	1.76	inches	/	31	davs
NH4	0.05677		inches			
NO3	0.05677	1.76				
TIME	366	1.70	T11C11G2	/	JI	aays
1 11111	300					



## GROUP L: PARAMETERS, CONSTANTS AND TIME-VARIABLE FUNCTIONS (PCFILNA)

Inputs required for this group include:

- 1. number of 2-D parameters
- 2. scale factors for 2-D parameters
- 3. parameter names
- 4. actual 2-D parameters
- 5. number of 3-D parameters
- 6. scale factors for 3-D parameters
- 7. parameter names
- 8. actual 3-D parameters
- 9. number of constants
- 10. actual constants
- 11. number of time-variable functions (tvfs)
- 12. tvf name and the number of time-breaks required to specify the tvf
- 13. actual tyfs
- 14. number of kinetic specific input file names
- 15. file names

#### L1. The Number of 2-Dimensional Parameters

80	-	
Comment	_	
FORMAT (A80)		
Comment	=	Comment line (ignored by RCA)
10		
NPARM2D		
FORMAT(I10)		

NPARM2D = number of 2-dimensional (or depth-independent) parameters

If there are no 2-D parameters to be read, skip over the next three input types and proceed with input type L5.



#### L2. <u>2-D Scale Factors</u>

Comment FORMAT (A80)

Comment ine (ignored by RCA)

<u>10 20 80</u> <u>PSCAL(1) PSCAL(2) --- PSCAL(NPARM2D)</u> FORMAT(8F10.0)

PSCAL(I) = scale factor for the Ith 2-D parameter set

#### L3. Parameter Name

20 PNAME FORMAT(A20)

PNAME = alphanumeric name for parameter set to be read

#### L4. <u>2-D Parameters</u>

PARAM2D(1,NY,I) PARAM2D(2,NY,I) --- PARAM2D(NX,NY,I) FORMAT(8F10.0)

PARAM2D(IX,IY,I) = value of the Ith parameter in segment or grid cell (IX,IY)

The parameters for the Ith parameter set are read a column at a time. The equivalent FORTRAN read statements would be:

DO I = 1,NPARM2D DO IY = 1,NY READ \*, (PARAM2D(IX,IY,I), IX = 1, NX) ENDDO ENDDO



#### L5. The Number of 3-Dimensional Parameters

Comment FORMAT (A80)

Comment ine (ignored by RCA)

<u>5</u> NPARM3D FORMAT(10)

NPARM3D = number of 3-dimensional (or depth-dependent) parameters

If there are no 3-D parameters to be read, skip over the next three input types and proceed with input type L9.

#### L6. 3-D Parameter Scale Factors

Comment FORMAT (A80)

Comment ine (ignored by RCA)

10 20 80
PSCAL(1) PSCAL(2) --- PSCAL(NPARM3D)
FORMAT(8F10.0)

PSCAL(I) = scale factor for the Ith 3-D parameter set

#### L7. Parameter Name

20 PNAME FORMAT(A20)

PNAME = alphanumeric name for parameter set to be read



#### L8. <u>3-D Parameters</u>

10	20	80
PARAM3D(1,1,1,I)	PARAM3D(2,1,1,I)	PARAM3D(NX,1,1,I)
	10	80
PARAM3D(1,NY,NZ	,l)	PARAM3D(NX,NY,NZ,I)
FORMAT(8F10.0)		

PARAM3D(IX,IY,IZ,I) = value of the Ith parameter

M3D(IX,IY,IZ,I) = value of the Ith parameter in segment (IX,IY,IZ)

The parameters for the Ith parameter set are read by layer, by column. The equivalent FORTRAN read statement would be:

```
DO I = 1,NPARM3D

DO IZ = 1,NZ

DO IY = 1,NY

READ *,(PARAM3D(IX,IY,IZ,I), IX = 1, NX)

ENDDO

ENDDO

ENDDO
```

Input types L7 and L8 are read for each parameter set, from 1 through NPARM3D.

#### L9. Number of Constants

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 NCONS FORMAT(I10)

NCONS = number of constants to be read

If no constants are to be read, set NCONS equal to 0 and continue with input type L11.



L10. Constants

CNAME(NOCONS-1) CNAME(NOCONS) CONST (NOCONS-1) CONST (NOCONS)

FORMAT(8A10/8F10.0)

CNAME(1) = name of the  $I^{th}$  constant CONST(I) = value of the  $I^{th}$  constant

The specification of CNAME is optional, but by specifying alphanumeric text it facilitates editing the constants section of the input file.

#### L11. Number of Time-Variable Functions (TVFs)

Comment FORMAT (A80)

Comment ine (ignored by RCA)

10 20 NOFUNC ITVFPLOPT FORMAT(2I10)

NOFUNC = number of time-variable functions to be read

ITVFPLOPT = step function or piecewise linear interpolation option

= 0, use step function

= 1, use piece wise linear interpolation

Data associated with Data Types L12 and L13 will be read NOFUNC times; once for each time-variable function required by the model.

L12. TVF Name and the Number of TVF Time Breaks
(Note if NOFUNC = 0, no input is required for L12 and L13.)

Comment FORMAT (A80)



Comment ine (ignored by RCA)

10	20	30
PNAME	NOBRK	TWARPTWF
FORMAT (A10.I10.6X	A4)	

PNAME = name of the time-variable function (tvf)

NOBRK = number of time breaks required to specify the tvf TWARPTWF = units to be used for the time breaks in the tvf.

SECS or secs,MINS or mins,HRS or hrs,DAYS or days.

#### L13. <u>Time-Variable Function</u>

VALT(I) = value of the function at time T(I)

T(I) = time in seconds (or units specified by TWARPTVF).

Note: Unlike previous versions of RCA all tvfs do not have to use the same time breaks  $(\Gamma(I))$ .

#### L14. Number of Miscellaneous Input Files to be Used by the Kinetic Subroutine

80
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 NOKINFILNA FORMAT (I10)

NOKINFILNA = number of file names to be read



#### L15. File Names

KINFILNA(I)
FORMAT(A40)

KINFILNA(I) =

complete path length and file name for kinetic subroutine input file I. The number of file names and the order in which they are specified is determined by the kinetic subroutine being used.

Table 10 presents a sample parameter, constant, tvf input file for a model with 10 cells in the x-direction, 5 cells in the y-direction, and 2 vertical layers with two 2-D parameters, one 3-D parameter, 44 constants, 1 time-variable function and 2 kinetic subroutine specific input files.



TABLE 10. EXAMPLE OF A PARAMETER, CONSTANTS AND TIME-VARIABLE FUNCTION INPUT FILE-PCFII NA

	J <b>FILNA</b> N2DPARAM								
С	2 Scale1	Scale2							
С	0.3048	1.0	oefficient						
C		0.000	0.000	0.000	0.000	0.000	0.000	0.000	
	0.000	0.787	0.787	0.850	0.880	0.925	1.250	1.150	
	0.000	0.787	0.787	0.850	0.880	0.920	1.170	1.120	
	0.000	0.787	0.787	0.840	0.870	0.900	0.980	1.100	
	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	
С	Kl - mass 0.0	trasnfe:	r coefficient	t (reaer	ation coeff	ficient) 0.0	0.0	0.0	
	0.0	0.0 1.5	1.5	1.5	1.5	1.0	1.0	1.0	
	1.5	0.0	1.5	1.5	1.5	1.0	1.0	1.0	
	1.5	0.0	1.5	1.5	1.5	1.0	1.0	1.0	
	1.5 0.0 0.0	0.0 0.0 0.0	0.0	0.0	0.0	0.0	0.0	0.0	
C N3DPARAM  1 number of 3D							parameters		
С	SCALE 1.0E-00								
С	SS (mg/L) 0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0 15.	15.	15.	14.	layer 12.	10.	10.	
	10.	0.0 15.	15.	15.	14.	12.	10.	10.	
	10.	0.0 15.	15.	15.	14.	12.	10.	10.	
	10.	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0 18.	18.	18.	16.	layer 14.	12.	11.	
	11.	0.0 18.	18.	18.	16.	14.	12.	11.	
	11.	0.0 18. 0.0	18.	18.	16.	14.	12.	11.	
	11. 0.0 0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
С	NCONS 20				number o	of constar	nts		
	AGOPT 0.	KAOPT 1.	KEOPT 2.	Unused	Unused		K1BETA1	K2BETA2	
	K1C 2.500	K1T 1.068	IS1 150.000	KMN1 0.010	KMP1 0.001	KMS1 0.020	K1RB 0.075	K1RG 0.0	
	K1RT	K1GZC	K1GZT	CCHL1	CPR11	CPR12	CPR13	CNR11	
	1.047 CNR12	0.100 CNR13	1.10 CSR11	30.0 CSR12	40.0 CSR13	0.0 TOPT2	0.0 K2BETA1	5.670 K2BETA2	
	0.0	0.0	5.0	10.0	0.0	22.	.004	.006	
	K2C	K2T	IS2 350.0	KMN2 0.010	KMP2 0.001	KMS2 0.002	K2RB 0.075	K2RG 0.	
	2.400 K2RT	1.068 K2GZC	K2GRT	CCHL2	0.001	0.002	0.075	0.	
С	1.047	0.120 VPWLOPT	1.100	80.0					
С	1 PNAME	1	TWARPTVF		number	of time f	functions		
_	ITOT	13	DAYS		DAILY RAD		21.0	0.0	
	118. 418.	0. 120.	168. 468.	11. 151.	218. 518.	59. 181.	318. 468.	90. 212.	
	418.	243.	318.	273.	218.	304.	168.	335.	
С	118. NOKINFILNA	365.							
	2								





#### **GROUP M: INITIAL CONDITIONS**

Inputs required for this group include:

- 1. sigma level or standard level input option
- 2. initial conditions

M1. Option to Read Initial Conditions Using Sigma Levels or Standard Lev
--

Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

10
ICOPT
FORMAT(I0)

ICOPT = sigma-level or standard level input option = 0, use sigma-level = 1, use standard level

Sigma-Level Initial Conditions (ICOPT=0)

M2. <u>Initial Conditions (or Initial Solution Estimates)</u>

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

FORMAT(10X,7F10.0)



CARAY(IX,IY,IZ,ISYS)= initial condition for segment grid cell (IX,IY,IZ) for system ISYS

The initial conditions are read by system, by layer, by y-direction. The equivalent read statement would be:

```
DO ISYS = 1,NOSYS
DO IZ = 1,NZ
DO IY = 1,NY
READ*, (CARAY(IX,IY,IZ,ISYS), IX = 1,NX)
ENDDO
ENDDO
ENDDO
ENDDO
```

Standard Level Initial Conditions (ICOPT=1)

M2. Number of Standard Levels

Comment FORMAT (A80)

Comment | Comment line (ignored by RCA)

10 NLVLS FORMAT(I10)

NLVLS = number of standard levels at which initial conditions are

defined

M3. Standard Level Depths

<u>10 20 80</u> <u>SLDEPTH(1) SLDEPTH(2) . . . SLDEPTH(NLVLS)</u>

SLDEPTH(1) = the depth in meters of the  $I^{TH}$  standard level

M4. <u>Initial Conditions at Standard Levels</u>



CARAYSL(IX,IY,IZ) = initial condition at standard depth level IZ for segment grid cell (IX,IY)



## **APPENDIX A**

# INTEGRATED EUTROPHICATION AND SEDIMENT NUTRIENT FLUX MODELS

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=	of NH <sub>3</sub> and NO <sub>2</sub> +NO <sub>3</sub> .	59



#### 1.0 KINETIC FRAMEWORK FOR THE INTEGRATED EUTROPHICATION MODEL

#### 1.1 INTRODUCTION

This portion of the RCA Users Guide describes an integrated eutrophication/sediment nutrient flux modeling framework, available with the Public Domain release of RCA. In addition, the range in kinetic coefficients used in a number of eutrophication studies performed by HydroQual are provided as a reference.

#### 1.1.1 Conservation of Mass

The modeling framework described in this document is based upon the principle of conservation of mass. The conservation of mass accounts for all of a material entering or leaving a body of water, transport of the material within the water body, and physical, chemical and biological transformations of the material. For an infinitesimal volume oriented along the axis of a three-dimensional coordinate system, a mathematical formulation of the conservation of mass may be written:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left( E_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left( E_y \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left( E_z \frac{\partial c}{\partial z} \right) - U_x \frac{\partial c}{\partial x} - U_y \frac{\partial c}{\partial y} - U_z \frac{\partial c}{\partial z}$$
(1-1)
dispersive transport
$$advective transport$$

$$\pm S(x, y, z, t)$$
 +  $W(x, y, z, t)$   
sources or sinks external inputs

where:

c = concentration of the water quality variable  $[M/L^3]$ ,

t = time [T],

E = dispersion (mixing) coefficient due to tides and density and velocity gradients ( $L^2/T$ ),

U = advective velocity (L/T),

S = sources and sinks of the water quality variable, representing kinetic interactions  $(M/L^3-$ 

T

W = external inputs of the variable c  $(M/L^3-T)$ ,

x,y,z = longitudinal, lateral and vertical coordinates,

M,L,T = units of mass, length and time, respectively.

The modeling framework is made up of two components: (1) the transport due to freshwater flow in riverine systems and/or tidal, meteorological and density-driven currents in esturaine and coastal systems, and (2) the kinetic interactions between variables and the external inputs. Freshwater flow and/or density-driven currents and tidally and wind induced mixing are responsible for the movement of the water quality constituents within the waterbody.

External inputs of nutrients and oxygen-demanding material are derived from numerous sources, including: municipal and industrial discharges, combined sewer overflows (CSOs), storm sewer overflows (SSOs), natural surface runoff, and atmospheric deposition to the water surface of the waterbody.



The kinetics control the rates of interactions among the water quality constituents. Ideally, in a modeling effort, they should be independent of location per se, although they may be functions of exogenous variables, such as temperature and light, which may vary with location.

Analytical solutions are not available for partial differential equations of the form of Equation 1-1 except for the simplest cases. Instead, numerical methods are utilized to solve these mass balance equations. A specific method of solution employed in a majority of water quality modeling frameworks is known as the finite difference technique. First, the estuary is divided into finite volumes. Then a finite difference approximation of Equation 1-1 is applied to the i<sup>th</sup> finite volume or segment, resulting in an equation of the form (see Thomann and Mueller, 1987):

$$V_{i} \frac{dc_{i}}{dt} = \sum_{j=1}^{n} R_{ij} (c_{j} - c_{i}) + \sum_{k=1}^{n} Q_{ki} c_{k} - \sum_{m=1}^{n} Q_{im} c_{i} \pm S_{i} + W_{i}$$

$$i = 1, 2, ... n \text{ (where } n = \text{number of segments)}$$
(1-2)

where

 $V_i$  = volume of segment i (L<sup>3</sup>),

 $c_i$  = concentration of the water quality variable in the i<sup>th</sup> segment,  $(M/L^3)$ ,

 $R_{ij}$  = exchange between segment i and j resulting from dispersive mixing, (L<sup>3</sup>/T),

 $Q_{ki}$  = net advective flow entering segment i from segment k,  $(L^3/T)$ ,

 $Q_{im}$  = net advective flow leaving segment i and going to segment m,  $(L^3/T)$ ,

 $S_i$  = sources and sinks, in segment i representing kinetic interactions, (M/T),

 $W_i$  = external inputs to segment i (M/T).

The exchange coefficients and advective flows are computed from

$$R_{ij} = \frac{E_{ij} A_{ij}}{L_{ij}} \tag{1-3a}$$

and

$$Q_{ij} = A_{ij} U_{ij}$$
 (1-3b)

respectively, where  $E_{ij}$  is the dispersion coefficient, representing the overall phenomenon of mixing due to temporal variations in the tidal velocity, lateral and vertical gradients in velocity, and density differences within the water body;  $A_{ij}$  is the cross-sectional area of the ij interface;  $L_{ij}$  is the characteristic length defined as  $(L_i + L_j)/2$ ; and  $U_{ij}$  is the net advective velocity from segment i to j. The term  $S_i$ , the sources and sinks of material in segment i, represents the kinetic interactions (physical, chemical and biological) occurring within the segment. These interactions may be functions only of the variable under consideration, for example, the first order decay of organic material. Alternately, they may involve the interactions between other variables, e.g., the first order feed-forward interaction between the oxidation of organic carbon (BOD) and dissolved oxygen, or the more complex interactions between phytoplankton biomass and nutrients, which involve non-linear feed-forward and feed-back interactions. The term  $W_i$  represents the external inputs of material into segment i, including point and nonpoint source loads, CSO loads, and/or atmospheric loads.



Mass balance equations in the form of Equation 1-2 are formulated for each segment in the estuary and for each state-variable included in the modeling framework. This results in  $n \times m$  simultaneous finite difference equations to be solved, where n is the number of segments and m is the number of state-variables.

#### 1.1.2 Choice of State Variables

An important criterion for the inclusion of variables in a modeling framework is the existence of adequate field data for calibration/verification of the variable, as well as the importance of the variable in the processes being considered. The kinetic framework employed of the integrated eutrophication is based on the LIS 3.0 eutrophication model developed for the Long Island Sound Study (HydroQual, Inc. 1991), the Massachusetts Bays Eutrophication Model (BEM) developed for the Massachusetts Water Resources Authority (MWRA) and the modeling effort of the Chesapeake Bay system (Cerco and Cole, 1995) and utilizes the following 26 state variables:

- 1. salinity (S)
- 2. phytoplankton carbon winter assemblage (Pc1)
- 3. phytoplankton carbon summer assemblage (P<sub>c2</sub>)
- 4. phytoplankton carbon fall assemblage  $(P_{c3})$
- 5. refractory particulate organic phosphorus (RPOP)
- 6. labile particulate organic phosphorus (LPOP)
- 7. refractory dissolved organic phosphorus (RDOP)
- 8. labile dissolved organic phosphorus (LDOP)
- 9. algal phosphorus + dissolved inorganic phosphorus (PO<sub>4</sub>T)
- 10. refractory particulate organic nitrogen (RPON)
- 11. labile particulate organic nitrogen (LPON)
- 12. refractory dissolved organic nitrogen (RDON)
- 13. labile dissolved organic nitrogen (LDON)
- 14. algal nitrogen + ammonia nitrogen (NH<sub>4</sub>T)
- 15. nitrite + nitrate nitrogen (NO<sub>2</sub>+NO<sub>3</sub>)
- 16. biogenic silica unavailable (SiU)
- 17. algal silica + available silica (SiT)
- 18. refractory particulate organic carbon (RPOC)
- 19. labile particulate organic carbon (LPOC)
- 20. refractory dissolved organic carbon (RDOC)
- 21. labile dissolved organic carbon (LDOC)
- 22. algal exudate dissolved organic carbon (ExDOC)
- 23. reactive particulate organic carbon (RePOC)
- 24. reactive dissolved organic carbon (ReDOC)
- 25. dissolved oxygen equivalents (O<sub>2</sub>\*)
- 26. dissolved oxygen (DO)

The kinetic equations discussed below incorporate these state variables and are designed to simulate the annual cycle of phytoplankton production, its relation to the supply of nutrients and its effect on dissolved oxygen. The calculation is based on formulating the kinetics which govern the interactions of the



biota and the various nutrient forms, and the application of these kinetics to the waterbody within the context of mass conservation equations.

#### 1.2 MODEL KINETICS

#### 1.2.1 General Structure

Salinity is included in the eutrophicaton modeling framework to enable verification that the transport structure of the hydrodynamic model (Blumberg and Mellor, 1987) is transferred to the water quality model properly. For salinity there are no reaction kinetics involved, i.e., they are conservative. There are no direct sources or sinks of salinity, other than via exchange with the model boundaries or via freshwater dilution resulting from wastewater treatment facility discharges, CSOs, etc. and from freshwater rivers draining into the waterbody.

Figure 1-1 presents the principal kinetic interactions for the nutrient cycles and dissolved oxygen. In the phosphorus system kinetics, dissolved inorganic phosphorus (DIP) is utilized by phytoplankton for growth. Phosphorus is returned from the phytoplankton biomass pool to the various dissolved and particulate organic phosphorus pools and to DIP through endogenous respiration and predatory grazing. The various forms of organic phosphorus are converted to DIP at a temperature dependent rate.

The kinetics of the nitrogen species are fundamentally the same as the kinetics of the phosphorus system. Ammonia and nitrite + nitrate are used by phytoplankton for growth. Ammonia is the preferred form of inorganic nitrogen for algal growth, but phytoplankton will utilize nitrite + nitrate nitrogen as ammonia concentrations become depleted. Nitrogen is returned from algal biomass and follows pathways that are similar to those of phosphorus. Organic nitrogen is converted to ammonia at a temperature dependent rate, and ammonia is then converted to nitrite + nitrate (nitrification) at a temperature and oxygen dependent rate. Nitrite + nitrate may be converted to nitrogen gas (denitrification) in the absence of oxygen at a temperature dependent rate.

Available silica is utilized by diatom phytoplankton during growth. Silica is returned to the unavailable silica pool during respiration and predation and must undergo mineralization processes before becoming available for phytoplankton growth.

Dissolved oxygen is coupled to the other state variables. The sources of oxygen considered are reaeration and algal photosynthesis. The sinks of oxygen are algal respiration, oxidation of detrital carbon and carbonaceous material from wastewater treatment plant effluents and nonpoint discharges, nitrification and SOD.

Organic carbon sources include anthropogenic inputs and the by-products of primary production and zooplankton grazing. The kinetic subroutine also incorporates two highly reactive organic carbon pools that can be used to represent organic carbon inputs from combined sewer overflows (CSOs) and/or waste water treatment plants (WWTPs) with poor treatment performance. The sink of organic carbon is via bacterial decomposition or oxidation. Specific details for the above reactions are presented below.



### 1.2.2 Phytoplankton Growth and Loss Kinetics

The current implementation of RCA permits the user to simulate up to three functional algal groups. They may represent a winter diatom group, a summer mixed assemblage, a fall mixed assemblage or they may represent a winter diatom group, a late spring/summer green group, and a late summer blue-green species (such as *Microcystis* or *Amabena*). The user, however, does have the option of implementing one, two, or three groups. In case, any kinetic framework employed for all three functional algal groups is the same, only the choice of model coefficients is different. It is convenient to express the kinetic source term for phytoplankton,  $S_P$ , as the difference between the phytoplankton growth rate,  $G_P$ , and the loss rate,  $D_P$ . That is:

$$S_{p} = (G_{p} - D_{p})P \tag{1-4}$$

where P is the phytoplankton biomass (in units of carbon), and where  $G_P$  and  $D_P$  have units (day<sup>-1</sup>). The balance between the magnitude of the growth rate and the loss rate (together with the transport and mixing) determines the rate at which phytoplankton mass is created (or lost) in each volume element.

The growth rate of a population of phytoplankton in a natural environment is a complicated function of the species of phytoplankton present and their differing reactions to solar radiation, temperature, and the balance between nutrient availability and nutrient requirements. In order to construct a growth function, a simplified approach is followed. Rather than consider the problem of different species and their associated environmental and nutrient requirements, the population is characterized as a whole by a measurement of the biomass of the phytoplankton present.

For single species, the direct measure of the population size is the number of cells per unit volume. Cell counts of a single species may be obtained fairly readily in a well-controlled laboratory environment. However, in naturally occurring populations, this measure may be somewhat ambiguous. It is often difficult to distinguish between viable and non-viable cells, and colonizing species tend to pose a problem because counts usually do not distinguish individual cells, and the sizes of the colonies are quite variable.

The sum of the numbers of each species, the total count, could be used to characterize biomass, but since cell size varies substantially, the pico-phytoplankton would dominate such an aggregation. To account for this, the total bio-volume, or wet weight of phytoplankton, assuming unit density, can be calculated using characteristic volumes for each identified species. Unfortunately, volumes can vary appreciably as a function of nutrient availability. Conversion to phytoplankton dry weight and carbon involves further species-dependent constants, which are also nutrient dependent, and, therefore, are subject to variation and uncertainty. Thus, although the use of phytoplankton dry weight or carbon concentration is an appealing solution to the issue of aggregation, it suffers from some practical difficulties.

An alternative approach to this problem is to measure a parameter which is characteristic of all phytoplankton, namely, chlorophyll-a (chl-a), and to use this as the aggregated variable. The principal advantages are that the measurement is direct, it integrates cell types and age, and it accounts for cell viability. The principal disadvantages are that it is a community measurement with no differentiation between functional groups (for example, diatoms or blue-green algae), and it is not necessarily a good measurement of standing crop in dry weight or carbon units, since the chlorophyll to dry weight and



chlorophyll to carbon ratios are variable, and non-active chlorophyll (phaeo-pigments) must be measured to determine viable chlorophyll concentrations.

As can be seen from the above discussion, no simple aggregate measurement is entirely satisfactory. From a historical and practical point of view, the availability of extensive chlorophyll-a data for many waterbodies essentially dictates its use as the aggregate measure of the phytoplankton population, or biomass, for calibration and verification purposes. However, for internal computations, the eutrophication model uses phytoplankton carbon as a measure of algal biomass. The reasons for choosing phytoplankton carbon, rather than chl-a as the internal state variable, are twofold. The first reflects the fact that measures of primary production (an important measure of carbon fixation or growth) are made in carbon units. The second reason is that the use of phytoplankton carbon greatly facilitates the model computation of oxygendemanding material deposited to the sediment bed via settling.

### 1.2.2.1 Standard Algal Growth Model

At the current time, HydroQual uses one of two algal growth model formulations. The first of these (to be referred to as the "standard" algal growth model formulation) dates back to the early work of DiToro, O'Connor, and Thomann on the Sacramento-San Joaquin River system (DiToro et al., 1971), the Great Lakes (DiToro and Matystik, 1980, DiToro and Connolly, 1980), and the Potomac Estuary (Thomann et al, 1974, Thomann and Fitzpatrick, 1982). The second algal growth model (to be referred to as the Laws and Chalup model) is based on the model developed by Laws and Chalup (1990) and applied by HydroQual (1995) to the Massachusetts Bays system.

To date, the standard model has been applied by HydroQual to more studies than has the Laws and Chalup model, but we feel there is merit in making both versions of the algal growth model available to the user. The details of the standard model will be presented first, followed by the Laws and Chalup model. These in turn will be followed by a description of the nutrient and dissolved oxygen kinetics.

With the choice of biomass units established, i.e., a carbon based system (mg C/L or gm C/m<sup>3</sup>), a growth rate, which expresses the rate of production of biomass as a function of the important environmental variables, temperature, light and nutrients, may be developed. The specific growth rate,  $G_P$ , is related to  $G_{Pmax}$ , the maximum growth rate at optimum light, temperature and nutrients, via the following equation:

$$G_{p} = G_{P_{max}} \cdot G_{T}(T) \cdot G_{I}(I) \cdot G_{N}(N)$$
temperature light nutrients (1-5)

where

 $G_T(T)$  is the effect of temperature,  $G_I(I)$  is the light attenuation given by

$$G_{I}(I) = g(I, f, H, k_{e})$$
 (1-6)

and  $G_N(N)$  is the nutrient limitation given by

$$G_{N}(N) = g(DIP, DIN, Si)$$
(1-7)



where T is the ambient water temperature; I is the incident solar radiation; f is the fraction of daylight; H is the depth of the water column; k<sub>e</sub> is the extinction or light attenuation coefficient; and DIP, DIN and Si are the available nutrients required for growth, dissolved inorganic phosphorus (ortho-phosphate), dissolved inorganic nitrogen (ammonia plus nitrite/nitrate) and dissolved available silica, respectively.

Initial estimates of  $G_{Pmax}$  are generally based upon the literature and/or previous modeling studies and are subsequently refined during the calibration process. During the simulation, the selected maximum growth rates are temperature corrected using spatially-dependent, time-dependent water column temperature values as computed by the hydrodynamic model. The temperature corrected growth rate is computed using one of the two following equations, which relates  $G_{Pmax}(T)$ , the growth rate at ambient temperature, T, to  $T_{Pmax}(T_{20})$  the growth rate at  $T_{20}(T_{20})$  the growth rate at  $T_{20}(T_{20})$  and  $T_{20}(T_{20})$  are  $T_{20}(T_{20})$  and  $T_{20}(T_{20})$  are  $T_{20}(T_{20})$  and  $T_{20}(T_{20})$  and  $T_{20}(T_{20})$  and  $T_{20}(T_{20})$  and  $T_{20}(T_{20})$  and  $T_{20}(T_{20})$  are  $T_{20}(T_{20})$  and  $T_{20}(T_{2$ 

$$G_{P_{max}}(T) = G_{P_{max}}(T_{20}) \theta^{T-20}$$
 (1-8a)

$$G_{P_{\text{max}}}(T) = G_{P_{\text{max}}} e^{-\beta_1 (T_{\text{opt}} - T)^2}$$
  $T \le T_{\text{opt}}$  (1-8b)

or

$$G_{P \max}(T) = G_{P \max} e^{-\beta_2 (T_{opt} - T)^2}$$
  $T > T_{opt}$  (1-8c)

where  $\theta$  is the Arrenhius temperature coefficient, and  $\beta_1$  and  $\beta_2$  are shaping coefficients. When using equations 1-8b and 1-8c to temperature correct  $G_{Pmax}$ ,  $T_{opt}$  has a much lower value for winter diatoms then would be used for the summer mixed assemblage. It is suggested to utilize the Arrenhius formulation when modeling one functional algal group and the shaped formulation when modeling two or more functional groups.

Figure 1-2 presents comparisons of the two temperature correction formulations. In Figure 1-2a, the normalized growth rates are compared for the Arrenhius (normalized to the 20°C growth rate versus the shaped formulation (normalized to the maximum growth rate at the optimum temperature) for a winter temperature optimum of 8°C and a summer temperature optimum of 24°C. Figure 1-2b presents a similar comparison but for "actual" growth rates of 1.7, 2.2, and 3.0 day for the Arrenhius, winter-shaped, and summer-shaped formulations. The temperature corrected growth rate is then adjusted to reflect effects due to ambient light and nutrient levels.

In the natural environment, the light intensity to which the phytoplankton are exposed is not uniformly at the optimum value. At the surface and near-surface of the air-water interface, photo-inhibition can occur due to high light intensities, while at depths below the euphotic zone, light is not available for photosynthesis due to natural and algal related turbidity. The light formulation included in the standard RCA modeling framework extends from a light curve analysis by Steele (1962) and accounts for both the effects of saturating light intensities and light attenuation through the water column. The depth-averaged light attenuated growth rate factor,  $G_{\rm I}({\rm I})$ , is presented in Equation 1-9 and is obtained by integrating the specific growth rate over depth:

where:



$$G_{I}(I) = \frac{e}{k_{e}H} \left[ exp \left( \frac{-I_{o}(t)}{I_{s}} e^{-k_{e}H} \right) - exp \frac{-I_{o}(t)}{I_{s}} \right]$$

$$(1-9)$$

e = 2.718

H = the water column depth or thickness of the water cell or segment (m),

 $k_e$  = the total extinction coefficient,  $k_{ebase} + k_c P_{chl-a}$  computed from the sum of the base, non-algal related, light attenuation,  $k_{ebase}$ , and the self-shading attenuation due to the ambient phytoplankton population  $k_c P_{chl-a}$  (m<sup>-1</sup>),

 $k_c$  = the algal related extinction coefficient per unit of chlorophyll (m<sup>2</sup>/mg chl-a),

 $P_{\text{chl-a}}$  = the ambient phytoplankton population as chlorophyll (mg chl-a/L), where  $P_{\text{chl-a}}$  =

 $P_c/a_{cchl}$ 

P<sub>c</sub> = the ambient phytoplankton population as carbon (mg C/L), a<sub>cchl</sub> = the ratio of algal carbon to algal chlorophyll (mg C/mg chl-a), I<sub>o</sub> = the incident light intensity at the segment surface (ly/day),

 $I_s$  = the saturating light intensity (ly/day).

The value of I<sub>o</sub> at the water surface, I<sub>surf</sub>, may be evaluated at any time, t, within the day using the following formula:

$$I_{\text{surf}}(t) = \frac{I_{\text{tot}}}{0.635 \,\text{f}} \sin \left[ \frac{\pi (t_{\text{d}} - t_{\text{sunrise}})}{\text{f}} \right]$$
 (1-10)

where

 $I_{tot}$  = total daily incident solar radiation (ly/day), f = fraction of daylight (daylight hours/24),

 $t_d$  = time of day,  $t_{sunrise}$  = time of sunrise

To account for the effect of variations of available light as a function of depth, the light intensity,  $I_{\rm o}$  (H), at any depth, H, is related to the incident surface intensity,  $I_{\rm surf}$  via the extinction coefficient,  $k_{\rm e}$  through the formula

$$I_o(H) = I_{surf} \exp^{-k_e H}$$
(1-11)

The effects of various nutrient concentrations on the growth of phytoplankton have been investigated, and the results are quite complex. As a first approximation to the effect of nutrient concentration on the growth rate, it is assumed that the phytoplankton population in question follows Monod growth kinetics with respect to the important nutrients. That is, at an adequate level of nutrient concentration, the growth rate proceeds at the saturated rate for the ambient temperature and light conditions. However, at low nutrient concentration, the growth rate becomes linearly proportional to nutrient concentration. Thus, for a nutrient with concentration  $N_j$  in the  $j^{th}$  segment, the factor by which the saturated growth rate is reduced in the  $j^{th}$  segment is  $N_j/(K_m + N_j)$ . The constant,  $K_m$ , which is called the Michaelis or half-saturation constant, is the nutrient concentration at which the growth rate is half the saturated growth rate. Since there are three nutrients, nitrogen, phosphorus and silica, considered in this



framework, the Michaelis-Menton expression is evaluated for each nutrient and the minimum value is chosen to reduce the saturated growth rate,

$$G_{N}(N) = Min\left(\frac{DIN}{K_{mN} + DIN}, \frac{DIP}{K_{mP} + DIP}, \frac{Si}{K_{mSi} + Si}\right)$$
(1-12)

Numerous mechanisms have been proposed which contribute to the death rate of phytoplankton: endogenous respiration, grazing by herbivorous zooplankton, sinking or settling from the water column and parasitization (Fogg, 1965). The first three mechanisms have been included in previous models for phytoplankton dynamics and they have been shown to be of general importance. For this version of the integrated eutrophication model, only endogenous respiration and settling have been explicitly included in the modeling framework. The effect of zooplankton grazing is included indirectly using a first-order temperature corrected algal loss rate.

The endogenous respiration rate of phytoplankton is the rate at which the phytoplankton oxidize their organic carbon to carbon dioxide per unit weight of phytoplankton organic carbon. Respiration is the reverse of the photosynthesis process, and as such, contributes to the loss rate of the phytoplankton population. If the respiration rate of the phytoplankton, as a whole, is greater than the growth rate, there is a net loss of phytoplankton carbon or biomass. The endogenous respiration rate has been shown to be temperature dependent (Riley et al., 1949) and historically has been included in eutrophication models using Equation 1-13a,

$$k_{PR}(T) = k_{PR}(20^{\circ}C) \cdot \theta_{PR}^{(T-20)}$$
 (1-13a)

where  $k_{PR}$  (20°C) is the endogenous respiration rate at 20°C, and  $k_{PR}$ (T) is the temperature corrected rate. The units of  $k_{PR}$  are day<sup>-1</sup>.

However, more recently the literature (Laws and Bannister, 1980, Laws and Chalup, 1991) suggests that algal respiration should be divided into two components - basal or resting respiration and respiratory losses associated with photosynthesis. This may be written mathematically as follows:

$$k_{pR}(T) = r_{\sigma}G_{p} + r_{b}\theta_{pR}^{T-20}$$
 (1-13b)

where  $r_g$  is the fraction of the algal growth ( $G_p$ ) lost to the energy cost of photosynthesis and  $r_b$  is the basal respiration rate. Note, the user can select either form of the respiration rate equation when performing a simulation. If the user wishes to use the first formulation (equation 1-13a) then set  $r_g$  equal to zero and use an appropriate value for  $r_b$  ( $\sim 0.1$ -0.3/day). If the user wises to use the latter form (equation 1-13b) then set  $r_g$  to a non-zero value (0.1-0.3) and use a lower value (0.01-0.03/day) for  $r_b$ .

The sinking or settling of phytoplankton is an important contribution to the overall mortality of the phytoplankton population, particularly in lakes and coastal oceanic waters. Published values of the sinking velocity of phytoplankton, mostly in quiescent laboratory conditions, range from 0.1 to 18.0 m/day. However, in some instances for certain species, such as dinoflagellates or buoyancy-retulating blue-greens, the settling velocity may be zero or negative. Furthermore, actual settling rates in natural waters are a complex phenomenon, affected by vertical turbulence, density gradients and the physiological state of the



different species of phytoplankton. An important factor determining the physiological state of algae is nutrient availability. Bienfang et al. (1982) measured sinking rate response of four marine diatoms to depletion of nitrate, phosphate and silicate. All four species showed significant increase in sinking rate under conditions of silica depletion; one species showed increased settling rate under nitrate limitation. An analysis of field experiments by Culver and Smith (1989) indicated that low concentrations of nitrate, as well as light availability, affected diatom settling rates. Although the effective settling rate of phytoplankton is greatly reduced in a relatively shallow, well-mixed river or estuary, due to vertical turbulence, it still can contribute to the overall mortality of the algal population. In addition, the settling phytoplankton can be a significant source of nutrients to the sediments and can play an important role in the generation of SOD. For these reasons, a temperature- dependent term representing phyto-plankton settling has been included in the algal mortality expression, and may be written as follows:

$$\mathbf{k}_{\mathrm{sP}} = \left[ \frac{\mathbf{V}_{\mathrm{sPb}}}{\mathbf{H}} + \frac{\mathbf{V}_{\mathrm{sPn}}}{\mathbf{H}} \cdot \left( 1 - \mathbf{G}_{\mathrm{N}}(\mathbf{N}) \right) \right] \cdot \boldsymbol{\theta}_{\mathrm{base}}^{(\mathrm{T}-20)}$$
(1-14)

where  $k_{sP}$  is the net effective algal loss rate due to settling (day<sup>-1</sup>),  $v_{sPb}$  is the base settling velocity of phytoplankton (m/day),  $v_{sPn}$  is the nutrient dependent settling rate, (m/day),  $G_N(N)$  is defined by Equation 1-12, and H is the depth of the segment, (m).

Zooplankton grazing may, depending upon time of the year and zooplankton biomass levels, be an important loss rate for phytoplankton. The loss term used to represent zooplankton grazing is as follows:

$$k_{grz}(T) = k_{grz}(20^{\circ} C) \cdot \theta_{grz}^{(T-20)}$$
 (1-15)

where  $k_{grz}(T)$  is the temperature corrected loss rate due to zooplankton grazing and  $k_{grz}(20^{\circ}\text{C})$  is the predation rate at 20°C. The units of  $k_{grz}$  are day<sup>-1</sup>.

The total loss rate for phytoplankton is the sum of the three loss rates described above:

$$D_{P} = k_{PR}(T) + k_{sP} + k_{grz}(T)$$
 (1-16)

This completes the specification of the growth and death rates for phytoplankton (for the standard algal growth model) in terms of the physical variables: light, temperature and available nutrients. Table 1-1 summarizes the equations and model coefficients used in the standard version of the eutrophicaton model.



#### TABLE 1-1. STANDARD PHYTOPLANKTON GROWTH EQUATIONS

#### Phytoplankton Net Growth Rate

$$S_{p} = \left(G_{P \max} \cdot G_{T}(T) \cdot G_{I}(I) \cdot G_{N}(N) - k_{PR}(T) - k_{SP} - k_{grz}(T)\right) \cdot P_{c}$$

#### Temperature Correction

Arrenhius Version

$$G_{P_{max}}(T) = G_{P_{max}} \theta_{P}^{(T-20)}$$

Optimum Temperature Version

$$G_{\text{Pmax}}(T) = G_{\text{Pmax}} e^{-\beta_1 (T - T_{\text{opt}})^2}$$

$$T \le T_{\text{opt}}$$

$$G_{P_{max}}(T) = G_{P_{max}}e^{-\beta_2 (T_{opt} - T)^2}$$
  $T > T_{opt}$ 

Murderkill River Model

#### Light Reduction

$$G_{I}(I) = \frac{e}{k_{o}H} \left[ exp \left( \frac{-I_{o}(t)}{I_{o}} e^{-k_{o}H} \right) - exp \frac{-I_{o}(t)}{I_{o}} \right]$$
 Is = 350 ly/d

$$k_e = k_{e_{hace}} + k_c \cdot a_{cchl} \cdot P_c$$

#### Nutrient Uptake

$$G_N(N) = Min\left(\frac{DIN}{K_{mN} + DIN}, \frac{DIP}{K_{mP} + DIP}, \frac{Si}{K_{mSi} + Si}\right)$$

DIN = dissolved inorganic nitrogen =  $NH_4 + NO_2 + NO_3$ ,

DIP = dissolved inorganic phosphorus (PO<sub>4</sub>),

Si = available silica

#### Algal Respiration

$$k_{_{PR}}\left(T\right) = k_{_{PR}}\left(20^{\circ}C\right) \cdot \theta_{_{PR}}{}^{_{(T-20)}}$$

or

$$k_{PR}(T) = r_{g}G_{P} + r_{b}\theta_{PR}^{(T-20)}$$

#### Algal Settling

$$\mathbf{k}_{sP} = \left[ \frac{\mathbf{V}_{sPb}}{\mathbf{H}} + \frac{\mathbf{V}_{sPn}}{\mathbf{H}} \cdot \left( 1 - \mathbf{G}_{N}(\mathbf{N}) \right) \right] \cdot \boldsymbol{\theta}_{base}^{(T-20)}$$



TABLE 1-1. STANDARD PHYTOPLANKTON NET GROWTH EQUATIONS (Continued)

# Zooplankton Grazing

 $k_{grz}(T) = k_{grz}(20^{\circ}C) \cdot \theta_{grz}^{(T-20)}$ 

# Exogenous Variables

<u>Description</u>	<u>Notation</u>
Total Extinction Coefficient	$k_{e}$
Base Extinction Coefficient	$k_{ebase}$
Total Daily Surface Solar Radiation	$I_{o}$
Temperature	T
Segment Depth	Н

Segment Depth			Н		Murdorkill
	Rate (	<u>Constants</u>			Murderkill River
		Winter	Summer		Model
<u>Description</u>	<u>Notation</u>	<u>Diatoms</u>	<u>Assemblage</u>	<u>Units</u>	Model
Maximum Specific Growth Rate at $T_{opt}$	$G_{P_{\text{max}}}$	1.7-2.5	2.0 - 3.0	day <sup>-1</sup>	2.5
Temperature Coefficient	$ heta_{ ext{P}}$	1.068	1.068		1.068
Temperature Optimum	$T_{opt}$	6-12	20 - 25	°C	25
Shaping parameters	$\beta_1, \beta_2$	0.003-0.006	0.003-0.006		0.004-0.006
Phytoplankton Self-Light Attenuation	$k_c$	0.017	0.017	m <sup>2</sup> /mg chl-a	0.017
Half-Saturation Constant for Nitrogen	$K_{mN}$	10.	10.	$\mu g N/L$	10
Half-Saturation Constant for Phosphorus	$K_{mP}$	1.	1.	µgP/L	1
Half-Saturation Constant for Silica	$K_{mSi}$	20.	2.	μgSi/L	20
Respiration Rate	$k_{PR}(20^{\circ}C)$	0.1-0.3	0.1-0.3	day <sup>-1</sup>	
Temperature Coefficient	$ heta_{ ext{PR}}$	1.047-1.068	1.047-1.068		1.068
Cost of Photosynthesis	$\mathbf{r}_{\mathrm{g}}$	0.2 - 0.3	0.2 - 0.3		0.3
Basal Respiration	$r_{ m b}$	0.01-0.03	0.01-0.03	/day	0.05
Base Algal Settling Rate	$v_{sPb}$	0.2-1.0	0.2-1.0	m/day	0.3 0.0
Nutrient Dependent Algal Settling Rate	$V_{sPn}$	0.5-1.0	0.5-1.0	m/day	
Temperature Coefficient	$ heta_{ m base}$	1.029	1.029		1.027
Loss Due to Zooplankton Grazing	$k_{grz}(20^{\circ}C)$	0.05-0.10	0.05-0.10	/day	0.025
Temperature Coefficient	$oldsymbol{ heta}_{ m grz}$	1.10	1.10		1.10
Carbon/Chlorophyll Ratio	$a_{ m cchl}$	30-60.	75-100.	mgC/mg chl-a	



#### 1.2.2.2 Laws-Chalup Algal Growth Model

The second algal growth model available in this release of RCA draws directly from Laws and Chalup (1990) and an earlier modeling framework developed by Shuter (1979). The following paragraphs provide an overview of the Laws-Chalup model. In the Laws-Chalup model, the carbon in the phytoplankton cell is considered to be found in one of four compartments: structural carbon (S), reservoir or storage carbon (R), carbon associate with the light reactions (photochemical reactions) of photosynthesis (L), or carbon associated with the dark reactions (carbohydrate production and protein and lipid synthesis) of photosynthesis (D). Hence, total cell carbon, C = S + R + L + D. Chlorophyll is assumed to exist only in the L portion of the cell. Nutrients (nitrogen, phosphorus, and silica) are found in the S, L, and D portions of the cell and are assumed to be found in the same ratios in each of these pools. R is assumed to consist entirely of C storage products (carbohydrates and lipids) and hence contains no nutrients. The fraction of C allocated to structural purposes (S/C) is assumed to be constant and independent of growth conditions.

The steady-state gross photosynthetic rate per cell  $(\rho)$  is described by

$$\rho = G_{prl} L I = G_{prd} D \tag{1-17}$$

where I is the incident irradiance;  $G_{prd}$  is the gross photosynthetic rate per unit D and is a constant; and  $G_{prd}$  is the gross rate of photosynthesis per unit L per unit light intensity and is a function of environmental conditions. Respiration losses are assumed to be described by

$$k_{PR} = k_{RB} + k_{RG} G_{prd} D \tag{1-18}$$

where  $k_{RB}$  is the basal respiration rate per cell, i.e., the rate required to maintain the cell in the absence of growth, and  $k_{RG}$  is the growth-rate-dependent respiration coefficient (Laws and Bannister, 1980). The substrate for respiration is assumed to come from the R pool.

From the foregoing assumptions, it follows that the rate of nutrient assimilation  $f_N$  is constrained by

$$\frac{\mathrm{d}}{\mathrm{dt}}(S+L+D) = W_{Nx} f_{N} \tag{1-19}$$

where  $W_{Nx}$  is the ratio of C to nutrient x (either nitrogen, phosphorus or silica). It also follows that

$$\frac{dC}{dt} = G_{prd} D - k_{RB} - k_{RG} G_{prd} D$$
(1-20)

Under conditions of balanced growth it must be true that for any component X of the cell,

$$\mu = \frac{1}{X} \frac{dX}{dt} \tag{1-21}$$

where  $\mu$  is the growth rate in units of inverse time. Combining Equations (1-20) and (1-21) yields



$$\mu C = G_{prd} D - k_{RB} - k_{RG} G_{prd} D$$
 (1-22)

Laws and Chalup also define the assumptions and conditions under which a nutrient saturated version of Equation 1-22 can be developed. The nutrient saturated growth rate,  $\mu_{Pmax}$ , is of the form

$$\mu_{P_{max}} = \frac{G_{prd} (1 - k_{RG}) (1 - S/C) I}{I + G_{prd} / G_{prls}} - \frac{k_{RB}}{C}$$
(1-23)

where  $G_{prls}$  is the nutrient-saturated value of  $G_{prl}$ . Laws and Chalup then account for the relationship between light and  $G_{prls}$  by use of Equation (1-24).

$$G_{\text{prls}} = \frac{G_{\text{prlo}}}{1 + I/I_{\text{s}}} \tag{1-24}$$

where  $G_{prlo}$  is the value of  $G_{prls}$  when I = 0, and Is is the value of I when  $G_{prls} = 0.5G_{prlo}$ .

As described in Section 1.2.2.1 Standard Algal Growth Model, in the natural environment, the light intensity or incident irradiance, I, to which the phytoplankton are exposed is not uniformly at the optimum value. The variations in light exposure that phytoplankton are exposed to due to position in the water column and daily variations to solar radiation that were detailed in Section 1.2.2.1 also apply in the Laws-Chalup growth model. Equations (1-10) and (1-11) are used to determine the diurnal variation in solar radiation at the surface of the water column, given the total solar radiation, and its attenuation through the water column, respectively.

One additional parameterization that is incorporated in the Laws-Chalup formulation is photo-adaptation by phytoplankton. Phytoplankton have been shown to be able to adapt to variations in light intensity (Steemann Nielsen et al., 1962; Steemann Nielsen and Park, 1964; Morel et al. 1987). Experimental data have indicated that phytoplankton may take several hours to two to four days to adapt to changes in light intensity. Therefore, the value of I<sub>s</sub>, in Equation 1-24 is permitted to change as a function of the antecedent light history, according to the formula:

$$I_{s} = \left(I_{tot_{n-3}} + I_{tot_{n-2}} + I_{tot_{n-1}}\right)/3 \tag{1-25}$$

where:

 $I_{tot_{n-3}}$  = total solar radiation three days preceding current model day,  $I_{tot_{n-2}}$  = total solar radiation two days preceding current model day,  $I_{tot_{n-1}}$  = total solar radiation one day preceding current model day.

Note: the use of the photo-adaptation formula is optional. If the user wishes to include photo-adaptation then he or she should set the appropriate  $I_{sat}$  in the "Constants" section of the model input to zero. Otherwise, if a non-zero value for  $I_{sat}$  is specified then photo-adaptation is ignored the user specified value for  $I_{sat}$  is applied in equations (1-9) or (1-24).



The nutrient saturated growth rate is then temperature-corrected using spatially dependent, time-dependent values of ambient water column temperature as computed by the hydrodynamic model. The temperature-corrected growth rate is computed using either equation 1-8a or equations 1-8b and 1-8c. A principal difference between the winter diatom group and the summer assemblage is that the winter group has a much lower  $T_{\rm opt}$  than does the summer assemblage. The nutrient saturated, temperature-corrected growth rate is then adjusted to reflect effects due to nutrient levels, as described earlier (Equation 1-12). Table 1-2 presents the equations used for algal growth for the Law-Chalup version of algal growth.



#### TABLE 1-2. LAWS-CHALUP PHYTOPLANKTON GROWTH EQUATIONS

#### Phytoplankton Net Growth Rate

$$S_{_{D}} = (\mu_{_{Pmx}}(T, I) \cdot G_{_{N}}(N) - k_{_{RB}} - k_{_{SP}}(T) - k_{_{grz}}(T)) \cdot P_{_{C}}$$

#### Specific Growth Rate

$$G_n = \mu_{P_{max}}(T, I) \cdot G_N(N)$$

#### Nutrient Saturated Growth Rate

$$\mu_{\text{Pmax}}\left(T_{\text{opt}},I\right) = \frac{G_{\text{prd}} \cdot (1 - k_{\text{RG}}) \cdot (1 - S/C) \cdot I(z,t)}{G_{\text{prd}}/G_{\text{prlo}} + I(z,t) \; (1 + G_{\text{prd}}/I_{\text{s}}G_{\text{prlo}})} - k_{\text{RB}}$$

# Temperature Correction

$$\mu_{\mathrm{Pmax}}\left(T\right) = \mu_{\mathrm{Pmax}}\left(T_{\mathrm{opt}}\right) \cdot e^{-\beta_{l} \cdot \left(T - T_{\mathrm{opt}}\right)^{2}} \quad T \leq T_{\mathrm{opt}}$$

$$\mu_{\text{Pmax}}\left(T\right) = \mu_{\text{Pmax}}\left(T_{\text{opt}}\right) \cdot e^{-\beta_2 \cdot \left(T - T_{\text{opt}}\right)^2} \quad T > T_{\text{opt}}$$

### Light Attenuation

$$I(z,t) = I_{surf}(t) e^{-k_e z}$$

#### Average Light

$$I_{ave} = \frac{I_{surf}(t)}{k_{o}H} (1 - e^{-k_{e}H})$$

$$k_e = k_{e_{base}} + k_c \cdot a_{ChlC} \cdot P_c$$

$$I_{surf}(t) = \frac{I_{tot}}{0.635 \cdot f} sin \left( \frac{\pi \left( t_{d} - t_{sunrise} \right)}{f} \right)$$

$$I_s = (I_{tot_{n-3}} + I_{tot_{n-2}} + I_{tot_{n-1}})/3$$



# TABLE 1-2. LAWS-CHALUP PHYTOPLANKTON GROWTH EQUATIONS (CONTINUED)

### Chlorophyll to Carbon Ratio (a<sub>ChlC</sub>)

$$a_{ChlC} = \frac{1 - (1 - QF)(1 - \mu/\mu_{Pmax}) - S/C - (\mu + k_{RB}/C)/\left[(1 - k_{RG})G_{prd}\right]}{W_{CChl}}$$

#### Nutrient Uptake

$$G_{N}(N) = Min\left(\frac{DIN}{K_{mN} + DIN}, \frac{DIP}{K_{mP} + DIP}, \frac{Si}{K_{mSi} + Si}\right)$$

DIN = dissolved inorganic nitrogen =  $NH_3 + NO_2 + NO_3$ 

DIP = dissolved inorganic phosphorus

Si = available silica

#### Endogenous Respiration

$$k_{PR} = \frac{k_{RB} + k_{RG} \cdot \mu}{1 - k_{RG}}$$

$$\mu = G_N(N) \cdot \mu_{Pmax}$$

#### Algal Settling

$$k_{sP}(T) = \left(\frac{v_{sPb}}{H} + \frac{v_{sPn}}{H} \cdot (1 - G_{N}(N))\right) \cdot \theta_{sP}^{(T-20)}$$

#### Zooplankton Grazing

$$k_{grz}(T)\!=\!k_{grz}(20^{\circ}C)\!\cdot\!\theta_{grz}^{\phantom{grz}(T-20)}$$



TABLE 1-2. LAWS-CHALUP PHYTOPLANKTON GROWTH EQUATIONS (CONTINUED)

Exogenous Variables		
<u>Description</u>	<u>Notation</u>	<u>Units</u>
Total Extinction Coefficient	$k_{e}$	$m^{-1}$
Base Extinction Coefficient	$k_{ebase}$	$m^{-1}$
Total Daily Surface Solar Radiation	${ m I}_{ m tot}$	langleys/day
Temperature	Τ	°C
Segment Depth	Н	m
Fraction of Daylight	f	day
Time of Day	$t_d$	day
Time of Sunrise	$t_{\text{sunrise}}$	day

# Rate Constants

		Winter	Summer	
Description	<u>Notation</u>	<u>Diatoms</u>	<u>Assemblage</u>	<u>Units</u>
Gross photosynthetic rate per unit D	$G_{prd}$	2.5	3.0	day <sup>-1</sup>
Gross photosynthetic rate per unit L per unit light intensity in the limit of zero irradiance	$G_{\text{prlo}}$	0.28	0.28	m²/mol quanta
Quotient of nutrient to carbon ratios at relative growth rates of 0 and 1	QF	0.85	0.85	
Effect of Temperature below Topt on growth	$oldsymbol{eta}_1$	0.004	0.004	
Effect of Temperature above $T_{opt}$	$oldsymbol{eta}_2$	0.006	0.006	
Temperature Optimum	$T_{opt}$	8.	18.	°C
Phytoplankton Self-Shading Attenuation	$k_c$	0.017	0.017	m <sup>2</sup> /mg chl-a
Half-Saturation Constant for Nitrogen	$K_{mN}$	0.010	0.010	mgN/L
Half-Saturation Constant for Phosphorus	$K_{mP}$	0.001	0.001	mg P/L
Half-Saturation Constant for Silica	$K_{mSi}$	0.020	0.005	mg Si/L
Growth Related Respiration Coefficient	$k_{RG}$	0.28	0.28	
Basal Respiration Rate	$k_{RB}$	0.03	0.036	day <sup>-1</sup>
Base Algal Settling Rate	$v_{sPb}$	0.5	0.3	m/day
Nutrient Dependent Algal Settling Rate	$v_{sPn}$	1.0	0.7	m/day
Temperature Coefficient	$\boldsymbol{\theta}_{\mathrm{sP}}$	1.027	1.027	
Loss Due to Zooplankton Grazing	$k_{grz}$ (20°C)	0.1	0.1	day <sup>-1</sup>
Temperature Coefficient	$ heta_{ m grz}$	1.10	1.10	
Nutrient Saturated Carbon/Chlorophyll Ratio in L	$ m W_{CChl}$	40.	65.	mg C/mg chl-a
Ratio of Structural to Total Carbon	S/C	0.1	0.1	



#### 1.2.3 <u>Stoichiometry and Uptake Kinetics</u>

A principal component in the mass balance equations for the nutrient systems included in the eutrophication framework is the nutrient uptake kinetics associated with algal growth (as defined via equations (1-5) through (1-25)). In order to quantify the nutrient uptake it is necessary to specify the population stoichiometry in units of nutrient uptake per mass of population synthesized. For carbon as the unit of population biomass, the relevant ratios are the mass of nitrogen, phosphorus and silica per unit mass of carbon.

This version of the integrated eutrophication model includes two variable algal stoichiometry formulations as well as the more traditional constant stoichiometry formulation. The variable stoichiometry formulation allows internal algal nutrient levels to vary as a function of the external nutrient levels. This process is sometimes referred to as "luxury nutrient uptake". That is, when external nutrient levels are in surplus the internal nutrient to carbon ratio increases thereby allowing internal storage of nutrients. The reverse occurs when external nutrient levels are low and are approaching the nutrient half saturation constant. In this case, the internal nutrient to carbon ratios decrease and the algal cell can continue to grow at low external nutrient levels.

#### 1.2.3.1 Algal Stoichiometry and Uptake Kinetics - Standard Algal Growth Model

As mentioned above, two forms of variable nutrient stoichiometry are included in the integrated eutrophication model. The first is based on an emphirical formulation developed for the Chesapeake Bay model (Cerco, 1995). This formulation is presented graphically in Figure 1-3 for the carbon to phosphorus ratio from measurements collected in upper Chesapeake Bay.

A generalized variable stoichiometry formulation, based on the Chesapeake Bay model, may be written for a dissolved nutrient (DIX) as follows:

$$\frac{C}{X} = X_1 + (X_2 - X_1)e^{-X_3 \cdot DIX}$$
 (1-26)

where:

 $\frac{C}{x}$  = carbon to nutrient ratio,

 $X_1$  = nutrient saturated, carbon to nutrient ratio,

X<sub>2</sub> = nutrient limited, carbon to nutrient ratio (maximum),

X<sub>3</sub> = coefficient that determines the rate at which the carbon to nutrient ratio changes as a function of the ambient nutrient concentration, DIX,

DIX = dissolved concentration of available nutrient (either DIN, DIP, or DSi).



Table 1-3 lists the range in nitrogen, phosphorus and silica variable-stiochiometry coefficients used in previous modeling studies conducted by HydroQual.

TABLE 1-3. VARIABLE STOICHIOMETRY COEFFICIENTS - STANDARD ALGAL GROWTH MODEL

			Murderkill
	Winter <u>Assemblage</u>	Summer Assemblage	River Model
Nitrogen			
CRBN1 (mgC/mgN)	5.2-5.67	4-5.67	5.67
CRBN2 (mgC/mgN)	6.5-7.20	7.5-10.0	10.0
CRBN3 (L/mgN)	10-15	10-15	10.0
Phosphorus			
CRBP1 (mgC/mgP)	25-40	25-40	40.0
CRBP2 (mgC/mgP)	90	90	90.0
CRBP3 (L/mgP)	100-200	40-200	100.0
Silica			
CRBS1 (mgC/mgSi)	2.2-3.0	510.	7.5
CRBS2 (mgC/mgSi)	8-15	10-25	17.50
CRBS3 (L/mgSi)	12-30	5-10	7.5

#### 1.2.3.2 Algal Stoichiometry and Uptake Kinetics - Laws-Chalup Algal Growth Model

Lacking extensive measurements of the particulate forms of carbon, nitrogen, phosphorus and biogenic silica, many modeling studies have assumed that phytoplankton are comprised of carbon and nutrients which approximate Redfield ratios; i.e., 106C:16N:1P (atomic), under nutrient saturated conditions. However, while the use of Redfield ratios may be appropriate under nutrient saturated conditions, it has been shown (Anita et al., 1963; Caperon and Meyer, 1972; Chalup and Laws, 1990) that algae change their cellular composition or stoichiometry as a function of nutrient status. This is accounted for in the Laws/Chalup model via the following equations:

$$N_x : C = [QF + (1 - QF) (\mu/\mu_{P_{max}}] / W_{Cx}$$
  
=  $1/W_{Cx}$  when  $\mu = \mu_{P_{max}}$  (1-27)

and



$$Chl: C = \frac{1 - (1 - QF) (1 - \mu/\mu_{P_{max}}) - S/C - (\mu + k_{RB}/C)/[(1 - k_{RG}) G_{prd}]}{W_{chl}}$$

$$= \left\{1 - S/C - (\mu_{P_{max}} + k_{RB}C)/[(1 - k_{RG}) G_{prd}]\right\}/W_{chl} \text{ when } \mu = \mu_{P_{max}}$$
(1-28)

where:

 $N_{v}:C =$ the ratio of nutrient x (nitrogen, phosphorus or silica) to carbon,

QF =quotient of N<sub>x</sub>:C values at relative growth rates of 0 and 1,

the nutrient corrected growth rate ( $\mu = \mu_{P_{max}} GN(N)$ ),

 $W_{Cx} =$ the ratio of C to nutrient x in S, L, D, Chl:C =the ratio of chlorophyll-a to C in P,  $W_{Chl} =$ the ratio of C to chlorophyll-a in P.

The latter equation accounts for changes in the chlorophyll to carbon ratio both as a function of nutrient status and light. Equations 1-27 and 1-28 provide the equilibrium carbon to nutrient and carbon to chlorophyll ratios. However, as has been shown from experimental studies, there is a time period over which it takes the phytoplankton to reach new equilibrium conditions in response to changes in nutrient status and/or available light. This is accounted for by use of the following equations:

$$\frac{dN_x : C^n}{dt} = k_{eq} \left( N_x : C_{eq}^n - N_x : C^n \right)$$
(1-29)

$$N_x : C^{n+1} = N_x : C^n + dt \frac{dN_x : C^n}{dt}$$
 (1-30)

and

$$\frac{dChl:C^{n}}{dt} = k_{eq} \left(Chl:C^{n}_{eq} - Chl:C^{n}\right)$$
(1-31)

$$Chl: C^{n+1} = Chl: C^{n} + dt \frac{dChl: C^{n}}{dt}$$
(1-32)

where:

 $N_x:C^n, N_x:C^{n+1} =$ the nutrient to carbon ratios at time step n and n+1, respectively,

 $N_x:C_{eq}^n =$ the equilibrium nutrient to carbon ratio at time step n, as determined from

Equation 1-27,

a constant which determines the time to achieve equilibrium,

 $k_{eq} = Chl:C^n, Chl:C^{n+1} =$ the chlorophyll to carbon ratios at time step n and n+1, respectively,

the equilibrium chlorophyll to carbon ratio at time step n, as determined  $Chl:C^{n}_{_{e\alpha}}$ 

from Equation 1-28,

dt length of time step.

The Laws-Chalup algal growth model evaluates the nutrient to carbon and chlorophyll to carbon ratios to be used form the next time level based on the ratios at the current time level and the equilibrium ratios, determined from Equations 1-27 and 1-28, based upon environmental conditions at the current time level. A value of 1/day was chosen for k<sub>eq</sub>, based on the literature (Steeman Nielsen and Park, 1964; Anita et al., 1963; Caperon and Meyer, 1972). This corresponds to an equilibrium time of approximately 3 days. This



value has been "hard-wired" in the computer code. Table 1-4 contains the stoichiometric coefficients used in the Massachusetts Bays application of RCA.

TABLE 1-4 VARIABLE STOICHIOMETRY COEFFICIENTS -LAWS-CHALUP ALGAL GROWTH MODEL

	Winter Assemblage	Summer Assemblage
Nitrogen		
$W_{CN}$	5.67 (6.67 <sup>(1)</sup> - 16.2 <sup>(2)</sup> )	5.67 (6.67 <sup>(1)</sup> - 16.2 <sup>(2)</sup> )
Phosphorus		
$\mathrm{W}_{\mathrm{CP}}$	40.(47 <sup>(1)</sup> - 114 <sup>(2)</sup> )	40.(47 <sup>(1)</sup> - 114 <sup>(2)</sup> )
Silica		
$ m W_{csi}$	$2.5(2.94^{(1)} - 7.14^{(2)})$	$7.0(8.2^{(1)} - 20.^{(2)})$
QF	$0.85^{(1)}$	$0.85^{(1)}$
quotient of nutrient to carbon ratio at relative		
growth rates of 0 and 1		

<sup>(1)</sup> maximum C to nutrient ratio at nutrient-limiting conditions using Massachusetts Bays model coefficient of 0.85 for QF

Figure 1-4 presents a comparison of the carbon to nitrogen ratios obtained using the standard eutrophication variable stoichiometry foundation (Eqn. 1-26) using coefficients used in HydroQual studies versus that proposed by Laws and Chalup (Eqn. 1-27). It is important to note, however, that the coefficient set used by Laws and Chalup was for a single algal species and that a coefficient set that did not produce as sharp a curve was used by HydroQual in its Massachusetts Bay study (1995, 2003).

#### 1.2.3.3 Nutrient Cycling

Once the stoichiometric ratios have been determined, the mass balance equations may be written for the nutrients in much the same way as for the phytoplankton biomass. The principal processes determining the distribution of nutrients among the various pools are: the uptake of inorganic nutrients by phytoplankton for cell growth, the release of organic nutrients by algal respiration and predation processes, and the recycling of organic nutrients to inorganic forms via bacterial hydrolysis and mineralization.

In their work on Lake Huron and Saginaw Bay, Di Toro and Matystick (1980) proposed a nutrient recycle formulation that was a function of the localized phytoplankton population. Drawing from an analysis of available field data and citing the work of others (Hendry, 1977; Lowe, 1976; Henrici, 1938; Menon et al., 1972; and Rao, 1976) that indicated bacterial biomass increased as phytoplankton biomass increased, the mechanism chosen, saturating recycle, was a compromise. This compromise was between the conventional first-order temperature corrected mechanism and a second-order recycle mechanism, in which



<sup>&</sup>lt;sup>(2)</sup> maximum C to nutrient ratio at nutrient-limiting conditions using Laws-Chalup (1990) model coefficient f 0.35 for QF

the recycle rate is directly proportional to the phytoplankton biomass present, as indicated in pure culture, bacteria seeded laboratory studies (Jewell and McCarty 1971). The various relationships may be written:

First – order recycle: 
$$k(T) = k'(20^{\circ}C)\theta^{T-20}$$
 (1-33a)

Second – order recycle: 
$$k(T) = k''(20^{\circ}C)\theta^{T-20} \cdot P_c$$
 (1-33b)

Saturating recycle: 
$$k(T) = k'(20^{\circ}C)\theta^{T-20} \cdot \frac{P_c}{K_{mP_c} + P_c}$$
 (1-33c)

Saturating recycle permits second-order dependency at low phytoplankton concentrations, when  $P_c << K_{mPe}$ , where  $K_{mPe}$  is the half saturation constant for recycle. It also permits first-order recycle when the phytoplankton concentrations greatly exceed the half saturation constant. Basically, this mechanism employs a second order recycle that slows the recycle rate if the algal population is small, but does not permit the rate to increase continuously as phytoplankton concentrations increase. The assumption is that at higher population levels, other factors are limiting the recycle kinetics so that it proceeds at its maximum first-order rate.

#### 1.2.3.4 Organic Carbon

Seven organic carbon state variables are considered: reactive particulate organic (RePOC), reactive dissolved organic (ReDOC), labile dissolved (LDOC), refractory dissolved (RDOC), labile particulate (LPOC), refractory particulate (RPOC) and dissolved algal exudate (ExDOC). Reactive, labile and refractory distinctions are based upon the time scale of oxidation or decomposition. Reactive organic carbon decomposes on a time scale of days to a week or two and is meant to be used for CSO carbon and a portion of the organic carbon discharged from wastewater treatment plants; labile organic carbon decomposes on the time scale of several weeks to a month or two; refractory organic carbon decomposes on the order of months to a year. Reactive and labile organic carbon decompose primarily in the water column or else rapidly in the sediments. Refractory organic carbon decomposes much more slowly, almost entirely in the sediments.

Reactive particulate organic carbon (RePOC) is assumed to have a very high settling rate that is a function of RePOC itself (representing floculation). The underlying assumption is that at elevated concentrations floculations occurs, thereby enhancing the settling rate of this form of organic carbon. Equation 1-34 is used to determine the settling rates as a function of REPOC (Figure 1-5 illustrates REPOC

$$v=\min\left[v_{\text{max}}, v_{\text{min}} + (v_{\text{max}} - v_{\text{min}}) \left(\frac{\text{Re POC}}{C_{\text{ref}}}\right)^{\beta}\right]$$
 (1-34)

settling rate as a function of REPOC and the two model coefficients  $\beta$  and  $C_{ref}$ ). Information from settling column tests can be used to guide the selection of appropriate model coefficients, but it is important to (1) remember that settling column tests are usually conducted under quiescent conditions that may not occur in natural systems and (2) the choice of a maximum settling rate should be made remembering that the maximum rate may influence the integration step-size. For example, assuming a maximum rate of 50 m/day



a water column depth of 1 m and a ten layer sigma-level grid would require a time step of about 2.9 minutes or less to ensure numerical stability.

#### where

```
v = settling rate, (m/day)

v_{max} = maximum settling rate, (m/day)

v_{min} = maximum settling rate, (m/day)

RePOC = concentration of reactive (CSO) POC, (mg/L)

C_{ref} = reference concentration of RePOC, (mg/L)

\beta = power exponent for settling function
```

The principal sources of organic carbon are anthropogenic inputs and natural runoff, and detrital algal carbon, which is produced as a result of predation. Zooplankton take up and redistribute algal carbon to the organic carbon pools via grazing, assimilation, respiration and excretion. Since zooplankton are not directly included in the model, the redistribution of algal carbon by zooplankton is simulated by empirical distribution coefficients. An additional term, representing the excretion of DOC by phytoplankton during photosynthesis, is included in the model. This algal exudate is very reactive and has a time constant similar to the reactive DOC.

The decomposition of organic carbon is assumed to be temperature and bacterial biomass mediated. Since bacterial biomass is not directly included within the model framework, phytoplankton biomass is used as a surrogate variable. Table 1-5 presents the reaction rate terms and range of coefficients for each of the organic carbon pools considered in the model framework.



# TABLE 1-5. ORGANIC CARBON REACTION EQUATIONS (Numbering scheme refers to the variable list in Section 1.1.2)

#### Refractory Particulate Organic Carbon (RPOC)

$$S_{18} = f_{RPOC} \cdot k_{grz} (T) \cdot P_{c} - k_{18,20} \theta_{18,20}^{T-20} \cdot RPOC \cdot \frac{P_{c}}{K_{mP} + P_{c}} - \frac{v_{s18}}{H} \cdot RPOC$$

<u>Labile Particulate Organic Carbon (LPOC)</u>

$$S_{19} = f_{LPOC} \cdot k_{grz} (T) \cdot P_{c} - k_{19,21} \theta_{19,21}^{T-20} \cdot LPOC \cdot \frac{P_{c}}{K_{mP} + P_{c}} - \frac{v_{s19}}{H} \cdot LPOC$$

#### Refractory Dissolve Organic Carbon (RDOC)

$$\begin{split} S_{20} \ = & f_{RDOC} \cdot k_{grz} \ (T) \cdot P_c \ - k_{18,20} \ \theta_{18,20}^{\ T-20} \cdot RPOC \cdot \frac{P_c}{K_{mP_c} + P_c} \\ - k_{20,0} \ \theta_{20,0}^{\ T-20} \cdot RDOC \cdot \frac{P_c}{K_{mP_c} + P_c} \cdot \frac{DO}{K_{DO} + DO} \end{split}$$

#### Labile Dissolved Organic Carbon (LDOC)

$$\begin{split} S_{21} = & f_{LDOC} \cdot k_{grz} \cdot (T) \cdot P_c - k_{19,21} \, \theta_{19,21}^{-120} \cdot LPOC \cdot \frac{P_c}{K_{mP_c} + P_c} \\ & - k_{21,0} \, \theta_{21,0}^{-120} \cdot LDOC \cdot \frac{P_c}{K_{mP_c} + P_c} \cdot \frac{DO}{K_{DO} + DO} \cdot \frac{LDOC}{K_{mLDOC} + LDOC} \\ & - \frac{5}{4} \cdot \frac{12}{14} \cdot k_{15,0} \, \theta_{15,0}^{-120} \cdot NO_2 + NO_3 \cdot \frac{K_{NO_3}}{K_{NO_4} + DO} \end{split}$$

# TABLE 1-5. ORGANIC CARBON REACTION EQUATIONS (Numbering scheme refers to the variable list in Section 1.1.2) (Continued)

Algal Exudate Dissolved Organic Carbon (ExDOC)

$$S_{22} = f_{ExPP} \cdot G_P \cdot P_c - k_{22,0} \theta_{22,0}^{-T-20} \cdot ExDOC \cdot \frac{P_c}{K_{mP_c} + P_c} \cdot \frac{DO}{K_{DO} + DO} \cdot \frac{ExDOC}{K_{mLDOC} + ExDOC}$$

Reactive Particulate Organic Carbon (RePOC)

$$S_{23} = -k_{23,24} \theta_{23,24}^{\quad T-20} \cdot \text{Re POC} \cdot \frac{P_c}{k_{mp_c} + P_c} - \min \left[ v_{24\,\text{max}}, \, v_{24\,\text{min}} + \left( v_{24\,\text{max}} - v_{24\,\text{min}} \right) \left( \frac{\text{Re POC}}{C_{\text{ref}}} \right)^{\!\beta} \right] \cdot \text{Re POC}$$

Reactive Dissolved Organic Carbon (ReDOC)

$$S_{24} = -k_{23,24} \theta_{23,24}^{-T-20} \cdot Re \, POC \cdot \frac{P_c}{k_{mp_c} + P_c} \cdot k_{24,0} \theta_{24,0}^{-T-20} \cdot Re \, DOC \cdot \frac{P_c}{k_{mp_c} + P_c} \cdot \frac{DO}{K_{DO} + DO} \cdot \frac{Re \, DOC}{K_{mLDOC} + Re \, DOC}$$



TABLE 1-5. ORGANIC CARBON REACTION EQUATIONS (Numbering scheme refers to the variable list in Section 1.1.2)

Murderkill River Model

Description	<b>Notation</b>	<u>Value</u>	<u>Units</u>	
Phytoplankton Biomass	$P_c$	-	mgC/L	
Specific Phytoplankton Growth Rate	$G_{\mathrm{P}}$	Eq. 1-5	day <sup>-1</sup>	
Segment depth	Н	-	m	
Dissolved Oxygen	DO	-	${\rm mgO_2/L}$	
Half Saturation Constant for Phytoplankton Limitation	$K_{mPc}$	0.05	mgC/L	0.05
Fraction of Grazed Organic Carbon Recycle to:				
the LPOC pool	$ m f_{LPOC}$	0.30-0.40		0.40
the RPOC pool	$f_{RPOC}$	0.10-0.15		0.10
the LDOC pool	$\mathrm{f}_{\mathrm{LDOC}}$	0.35-0.45		0.40
the RDOC pool	$f_{RDOC}$	0.10-0.15		0.10
Note: the sum of $f_{LPOC} + f_{RPOC} + f_{LDOC} + f_{RDOC}$ must equal 1.0				
Fraction of Primary Productivity Going to the Algal Exudate DOC pool	$f_{\rm ExPP}$	0.10-0.15		0.10
Hydrolysis Rate for RPOC	$k_{18,20}$	0.007-0.01	day <sup>-1</sup>	0.01
Temperature Coefficient	$\boldsymbol{\theta}_{18,20}$	1.08		1.08
Settling Rate of RPOC	$v_{s18}$	0.5-1.0	m/day	0.3
Hydrolysis Rate for LPOC	k <sub>19,21</sub>	0.07-0.10	day <sup>-1</sup>	0.05
Temperature Coefficient	$\theta_{_{19,21}}$	1.08		1.08
Settling Rate of LPOC	$v_{s19}$	0.5-1.0	m/day	0.3
Oxidation Rate of RDOC	$k_{20,0}$	0.007-0.01	day <sup>-1</sup>	0.011
Temperature Coefficient	$\boldsymbol{\theta}_{20,0}$	1.08		1.08
Oxidation Rate LDOC	$k_{21,0}$	0.10-0.15	day <sup>-1</sup>	0.051
Temperature Coefficient	$\boldsymbol{\theta}_{21,0}$	1.08		1.08
Oxidation Rate of ReDOC	k <sub>22,0</sub>	0.25-0.35	day <sup>-1</sup>	0.05
Temperature Coefficient	$\boldsymbol{\theta}_{22,0}$	1.047		1.047
Oxidation Rate of ExDOC	$k_{23,0}$	0.1	day <sup>-1</sup>	0.05
Temperature Coefficient	$\theta_{23,0}$	1.08		1.08
Half Saturation for Oxygen Limitation	$k_{ m DO}$	0.2	${\rm mgO_2/L}$	0.2
Michaelis Constant for LDOC	$K_{mLDOC}$	0.1	mgC/L	0.1
Minimum RePOC settling rate	$v_{ m 24~min}$	0.5	m/day	not used
Enhanced RePOC settling rate (due to floculation)	${\rm V_{24max}}$	25	m/day	not used
Reference (or normalizing term)	$C_{Ref}$	10	mgC/day	not used
Power function	β	1.2		not used



#### 1.2.3.5 Phosphorus

The eutrophication model includes five principal phosphorus forms: labile and refractory dissolved organic (LDOP and RDOP, respectively), labile and refractory particulate organic (LPOP and RPOP, respectively), and DIP. Inorganic phosphorus is utilized by phytoplankton for growth and phosphorus is returned to the various organic and inorganic forms via respiration and predation. A fraction of the phosphorus released during phytoplankton respiration and predation is in the inorganic form and readily available for uptake by other viable algal cells. The remaining fraction released is in the dissolved and particulate organic forms. The organic phosphorus must undergo a mineralization or bacterial decomposition into inorganic phosphorus before it can be used by phytoplankton. Table 1-6 presents the reaction rate terms for each of the five phosphorus forms.

#### 1.2.3.6 Nitrogen

The kinetic structure for nitrogen is similar to that for the phosphorus system. Table 1-7 summarizes the terms used in the nitrogen system kinetics. During algal respiration and death, a fraction of the cellular nitrogen is returned to the inorganic pool in the form of NH<sub>3</sub>. The remaining fraction is recycled to the dissolved and particulate organic nitrogen pools. Organic nitrogen undergoes a bacterial decomposition, the end-product of which is NH<sub>4</sub>. Ammonia nitrogen, in the presence of nitrifying bacteria and oxygen, is converted to nitrite nitrogen and subsequently nitrate nitrogen (nitrification). Both ammonia and nitrate are available for uptake and are used in cell growth by phytoplankton; however, for physiological reasons, the preferred form is NH<sub>4</sub>. The ammonia preference term takes the following form:

$$\begin{split} \alpha_{\text{NH}_4} &= \text{NH}_4 \cdot \frac{\text{NO}_2 + \text{NO}_3}{\left(\text{K}_{\text{mN}} + \text{NH}_4\right) \cdot \left(\text{K}_{\text{mN}} + \text{NO}_2 + \text{NO}_3\right)} \\ &+ \text{NH}_4 \cdot \frac{\text{K}_{\text{mN}}}{\left(\text{NH}_4 + \text{NO}_2 + \text{NO}_3\right) \cdot \left(\text{K}_{\text{mN}} + \text{NO}_2 + \text{NO}_3\right)} \end{split} \tag{1-35}$$

The behavior of this equation for a Michaelis value, K<sub>mN</sub>, of 10 µgN/L, is illustrated on Figure 1-6. The behavior of Equation 1-35 is most sensitive at low values of ammonia or nitrate. For a given concentration of ammonia, as the available nitrate increases above approximately the Michaelis limitation, the preference for ammonia reaches a plateau. Also, as the concentration of available ammonia increases, the plateau occurs at values closer to unity, that is, total preference for ammonia. The process of nitrification in natural waters is carried out by aerobic autotrophs, *Nitrosomonas* and *Nitrobacter*, in particular. It is a two-step process with *Nitrosomonas* bacteria responsible for the conversion of ammonia to nitrite (NO<sub>2</sub>) and *Nitrobacter* responsible for the subsequent conversion of nitrite to nitrate (NO<sub>3</sub>). Essential to this reaction process are aerobic conditions. In order to reduce the number of state variables required in the modeling framework, it was decided to incorporate nitrite and nitrate together as a single state variable. Therefore, the process of nitrification is assumed to be approximated by a first-order reaction rate that is a function of the water column dissolved oxygen concentration and ambient temperature.



# TABLE 1-6. PHOSPHORUS REACTION RATES (Numbering scheme refers to the variable list in Section 1.1.2)

#### Refractory Particulate Organic Phosphorus (RPOP)

$$\begin{split} S_{5} &= a_{PC} \cdot f_{RPOP} \cdot \left(k_{PR}(T) + k_{grz}(T)\right) \cdot P_{c} - k_{5,7} \, \theta_{5,7}^{-7-20} \cdot RPOP \cdot \frac{P_{c}}{K_{mP_{c}} + P_{c}} \\ &- \frac{v_{s5}}{H} \cdot RPOP \end{split}$$

#### Labile Particulate Organic Phosphorus (LPOP)

$$\begin{split} \boldsymbol{S}_{6} &= \boldsymbol{a}_{PC} \cdot \boldsymbol{f}_{LPOP} \cdot \left(\boldsymbol{k}_{PR}(T) + \boldsymbol{k}_{grz} \right. \left(T\right)\right) \cdot \boldsymbol{P}_{c} - \boldsymbol{k}_{6,8} \left.\boldsymbol{\theta}_{6,8}^{-T-20} \cdot LPOP \cdot \frac{\boldsymbol{P}_{c}}{\boldsymbol{K}_{mP_{c}} + \boldsymbol{P}_{c}} \right. \\ &- \frac{\boldsymbol{v}_{s6}}{\boldsymbol{H}} \cdot LPOP \end{split}$$

### Refractory Dissolved Organic Phosphorus (RDOP)

$$\begin{split} S_{_{7}} \;\; &= \; a_{_{PC}} \cdot f_{_{RDOP}} \cdot \left(k_{_{PR}}(T) + k_{_{grz}} \; (T)\right) \cdot P_{_{c}} \, + \, k_{_{5,7}} \, \theta_{_{5,7}}{}^{_{T-20}} \cdot RPOP \cdot \frac{P_{_{c}}}{K_{_{mP_{_{c}}}} + P_{_{c}}} \\ &- k_{_{7,9}} \theta_{_{7,9}}{}^{_{T-20}} \cdot RDOP \cdot \frac{P_{_{c}}}{K_{_{mP_{_{c}}}} + P_{_{c}}} \end{split}$$

#### Labile Dissolved Organic Phosphorus (LDOP)

$$\begin{split} S_8 \;\; &= \; a_{PC} \, \cdot f_{LDOP} \, \cdot \left( k_{PR} \left( T \right) + \, k_{grz} \, \left( T \right) \right) \cdot P_c \, + \, k_{6,8} \, \theta_{6,8}^{\quad T-20} \cdot LPOP \, \cdot \frac{P_c}{K_{mP_c} \, + \, P_c} \\ \\ &- \, k_{8,9} \, \theta_{8,9}^{\quad T-20} \cdot LPOP \, \cdot \frac{P_c}{K_{mP_c} \, + \, P_c} \end{split}$$

# TABLE 1-6. PHOSPHORUS REACTION RATES (Continued)

#### Dissolved Inorganic Phosphorus (DIP)

$$\begin{split} S_9 &= a_{PC} \cdot f_{DIP} \cdot \left(k_{PR}(T) + k_{grz}(T)\right) \cdot P_c \\ &+ \left(k_{7,9} \cdot \theta_{7,9}^{T-20} \cdot RDOP + k_{8,9} \cdot \theta_{8,9}^{T-20} \cdot LDOP\right) \cdot \frac{P_c}{K_{mP_c} + P_c} \\ &- a_{PC} \cdot \left(1 - f_{ExPP}\right) \cdot G_P \cdot P_c \end{split}$$



TABLE 1-6. PHOSPHORUS REACTION RATES

Murderkill
River

(Cont.	inued)			Riv
	Notation	<u>Value</u>	<u>Units</u>	Mo
Phytoplankton Biomass	$P_c$	-	mgC/L	
Temperature Corrected Algal Respiration Rate	$k_{PR}(T)$	Eq. 1-11a	day <sup>-1</sup>	
Temperature Corrected Grazing Rate	$k_{grz}(T)$	Eq. 1-13	day <sup>-1</sup>	
Specific Phytoplankton Growth Rate	$G_{P}$	Eq. 1-5	day <sup>-1</sup>	
Phosphorus to Carbon Ratio	$a_{ m PC}$	Table 1-2	mgP/mgC	
Fraction of Primary Productivity Going to the Algal Exudate DOC pool	$\mathrm{f_{ExPP}}$	0.1		
Fraction of Respired and Grazed Algal Phosphorus Recycled to				
the LPOP pool	$ m f_{LPOP}$	0.25-0.35		0.
the RPOP pool	$f_{RPOP}$	0.10-0.15		0.
the LDOP pool	$\mathrm{f_{LDOP}}$	0.10-0.15		0.
the RDOP pool	$f_{RDOP}$	0.100.15		0.
the DIP pool	$\mathrm{f_{DIP}}$	0.20-0.45		0.
Note: the sum of $f_{LPOP} + f_{RPOP} + f_{LDOP} + f_{RDOP} + f_{DIP}$ must equal 1.0				
RPOP Hydrolysis Rate at 20°C	$k_{5,7}$	0.007-0.01	day <sup>-1</sup>	0.
Temperature Coefficient	$\boldsymbol{\theta}_{5,7}$	1.08		1.
RPOP Settling Rate	$V_{s5}$	0.5-1.0	m/day	0
LPOP Hydrolysis Rate at 20°C	$k_{6,8}$	0.085-0.10	day <sup>-1</sup>	0.
Temperature Coefficient	$\theta_{6,8}$	1.08		1.
LPOP Settling Rate	$V_{s6}$	0.5-1.0	m/day	0
RDOP Mineralization Rate at 20°C	k <sub>7,9</sub>	0.01-0.02	day <sup>-1</sup>	0.
Temperature Coefficient	$\theta_{7,9}$	1.08		1.0
LDOP Mineralization Rate at 20°C	$k_{8,9}$	0.1-0.2	day <sup>-1</sup>	0.0
Temperature Coefficient	$\theta_{80}$	1.08		1.



# TABLE 1-7. NITROGEN REACTION RATES (Numbering scheme refers to the variable list in Section 1.1.2)

### Refractory Particulate Organic Nitrogen (RPON)

$$\begin{split} S_{10} &= a_{NC} \cdot f_{RPON} \cdot \left( k_{PR}(T) + k_{grz} \, \left( T \right) \right) \cdot P_c - k_{10,12} \, \theta_{10,12}^{\phantom{10} T-20} \cdot RPON \cdot \frac{P_c}{K_{mP_c} + P_c} \\ &- \frac{V_{s10}}{H} \cdot RPON \end{split}$$

# Labile Particulate Organic Nitrogen (LPON)

$$\begin{split} S_{11} &= a_{NC} \cdot f_{LPON} \cdot \left( k_{PR}(T) + k_{grz}(T) \right) \cdot P_c - k_{11,13} \, \theta_{11,13}^{-7-20} \cdot LPON \cdot \frac{P_c}{K_{mP_c} + P_c} \\ &- \frac{V_{s11}}{H} \cdot LPON \end{split}$$

#### Refractory Dissolved Organic Nitrogen (RDON)

$$\begin{split} S_{12} &= a_{NC} \cdot f_{RDON} \cdot \left( k_{PR}(T) + k_{grz} \; (T) \right) \cdot P_c \; + k_{10,12} \, \theta_{10,12}^{\quad T-20} \cdot RPON \cdot \frac{P_c}{K_{mP_c} \; + P_c} \\ &- k_{12,14} \, \theta_{12,14}^{\quad T-20} \cdot RDON \cdot \frac{P_c}{K_{mP_c} \; + P_c} \end{split}$$

#### Labile Dissolved Organic Nitrogen (LDON)

$$\begin{split} S_{13} &= a_{NC} \cdot f_{LDON} \cdot \left( k_{PR}(T) + k_{grz}(T) \right) \cdot P_c + k_{11,13} \, \theta_{11,13}^{-T-20} \cdot LPON \cdot \frac{P_c}{K_{mP_c} + P_c} \\ & \qquad \qquad k_{13,14} \, \theta_{13,14}^{-T-20} \cdot LDON \cdot \frac{P_c}{K_{mP_c} + P_c} \end{split}$$



# TABLE 1-7. NITROGEN REACTION RATES (Continued)

#### Ammonia Nitrogen (NH<sub>4</sub>)

$$\begin{split} S_{14} &= a_{NC} \cdot f_{NH_4} \cdot \left(k_{PR}(T) + k_{grz} \cdot (T)\right) \cdot P_c \\ &+ \left(k_{12,14} \cdot \theta_{12,14}^{-T-20} \cdot RDON + k_{13,14} \cdot \theta_{13,14}^{-T-20} \cdot LDON\right) \cdot \frac{P_c}{K_{mP_c} + P_c} \\ &- a_{NC} \cdot \left(\alpha_{NH_4} \cdot \left(1 - f_{ExPP}\right) \cdot G_P \cdot P_c - k_{14,15} \cdot \theta_{14,15}^{-T-20} \cdot NH_4 \cdot \frac{DO}{K_{nitr} + DO} \right) \end{split}$$

#### Nitrite + Nitrate Nitrogen (NO<sub>2</sub>+ NO<sub>3</sub>)

$$\begin{split} S_{15} &= k_{14,15} \, \theta_{14,15}^{\phantom{15} T-20} \cdot \, NH_4 \, \cdot \, \frac{DO}{K_{nitr} \, + DO} - a_{NC} \, \cdot \left(1 - \alpha_{NH_4}^{\phantom{15}}\right) \cdot \\ & \left(1 - f_{ExPP}^{\phantom{15}}\right) \cdot G_P \, \cdot P_c \, - k_{15,0}^{\phantom{15}} \, \theta_{15,0}^{\phantom{15} T-20} \cdot \, NO_2 \, + \, NO_3 \, \cdot \, \frac{K_{NO_3}^{\phantom{15}}}{K_{NO_3} \, + \, DO} \end{split}$$



TABLE 1-7. NITROGEN REACTION RATES (Continued)

Murderkill River Model

(Contin	ideaj			Woder
<u>Description</u>	<u>Notation</u>	<u>Value</u>	<u>Units</u>	
Phytoplankton Biomass	$P_c$	-	mgC/L	
Temperature Corrected Algal Respiration Rate	$k_{PR}(T)$	cf Eq. 1-11a	day-1	
Temperature Corrected Grazing Rate	$k_{grz}(T)$	cf Eq. 1-13	day <sup>-1</sup>	
Specific Phytoplankton Growth Rate	$G_{P}$	cf Eq. 1-5	day <sup>-1</sup>	
Nitrogen to Carbon Ration	$a_{ m NC}$	cf Table 1-2	mgN/mgC	
Fraction of Primary Productivity Going to the Algal Exudate DOC pool	$f_{ExPP}$	0.1		
Fraction of Respired and Grazed Algal Nitrogen Recycled to				
The LPON pool	$f_{ m LPON}$	0.30-0.35		0.30
the RPON pool	$f_{RPON}$	0.10-0.15		0.10
the LDON pool	$f_{\rm LDON}$	0.125-0.15		0.15
the RDON pool	$f_{RDON}$	0.125-0.20		0.15
the NH <sub>4</sub> pool	$f_{NH4}$	0.15-0.35		0.30
Note: the sum of $f_{LPON}$ + $f_{RPON}$ + $f_{LDON}$ + $f_{RDON}$ + $f_{NH4}$ must equal 1.0				
RPON Hydrolysis Rate at 20°C	k <sub>10,12</sub>	0.007-0.01	day <sup>-1</sup>	0.01
Temperature Coefficient	$\theta_{10,12}$	1.08		1.08
RPON Settling Rate	$V_{s10}$	0.5-1.0	m/day	0.3
LPON Hydrolysis Rate at 20°C	k <sub>11,13</sub>	0.05-0.07	day <sup>-1</sup>	0.05
Temperature Coefficient	$\theta_{11,13}$	1.08		1.08
LPON Settling Rate	$V_{s11}$	0.5-1.0	m/day	0.3
RDON Mineralization Rate at 20°C	k <sub>12,14</sub>	0.0080.01	day <sup>-1</sup>	0.01
Temperature Coefficient	$\theta_{\scriptscriptstyle 12,14}$	1.08		1.08
LDON Mineralization Rate at 20°C	k <sub>13,14</sub>	0.085-0.10	day <sup>-1</sup>	0.05
Temperature Coefficient	$\theta_{13,14}$	1.08		1.08
Nitrification Rate at 20°C	k <sub>14,15</sub>	0.05-0.10	day <sup>-1</sup>	0.05
Temperature Coefficient	$\boldsymbol{\theta}_{14,15}$	1.08		1.08
Half Saturation Constant for Oxygen Limitation	K <sub>nitr</sub>	1.0	$\rm mg0_2/L$	1.0
Denitrification Rate at 20°C	$K_{15,0}$	0.05-0.4	day <sup>-1</sup>	0.05
Temperature Coefficient	$\theta_{15,0}$	1.045		1.045
Michaelis Constant for Denitrification	$K_{NO_3}$	0.1	${\rm mg0_{2/L}}$	0.1



Denitrification refers to the reduction of  $NO_3$  to  $N_2$  and other gaseous products such as  $N_2O$  and NO. This process is carried out by a large number of heterotrophic, facultative anaerobes. Under normal aerobic conditions found in the water column, these organisms utilize oxygen to oxidize organic material. However, under the anaerobic conditions found in the sediment bed or during extremely low oxygen conditions in the water column, these organisms are able to use  $NO_3$  as the electron acceptor. The process of denitrification is included in the modeling framework simply as a sink of nitrate. This can always occur in the anaerobic sediment layer. In the water column, however, denitrification should only occur under extremely low dissolved oxygen conditions. This is accomplished computationally by modifying the linear first-order denitrification rate by the expression  $K_{NO3}/(K_{NO3}+DO)$ . This expression is similar to the Michaelis-Menton expression; for concentrations of dissolved oxygen greater than 1 mg/L, the expression reduces denitrification to near zero, whereas for dissolved oxygen levels less than 0.1 mg/L, this expression permits denitrification to occur. Table 1-7 presents the state-variable equations for the six nitrogen forms utilized in the model framework.

#### 1.2.3.7 Silica

Two silica state-variables are considered: available (Si) and unavailable or particulate biogenic (SiU). Available silica is dissolved and is utilized by diatoms during growth for their cell structure. Unavailable or particulate biogenic silica is produced from diatom respiration and diatom grazing by zooplankton. Particulate biogenic silica undergoes mineralization to available silica or settles to the sediment from the water column. Table 1-8 presents the state-variable equations for the two silica forms utilized in the model framework.

### 1.2.3.8 Dissolved Oxygen

A by-product of photosynthetic carbon fixation is the production of dissolved oxygen. The rate of oxygen production and nutrient uptake is proportional to the growth rate of the phytoplankton, since its stoichiometry is fixed. An additional source of oxygen from algal growth occurs when the available ammonia nutrient source is exhausted and the phytoplankton begin to utilize the available nitrate. This additional oxygen source can be seen by comparing equations 1-36a and 1-36b (Morel, 1983).

$$106 \text{ CO}_{2} + 16 \text{ NH}_{4}^{+} + \text{H}_{2}\text{PO}_{4}^{-} + 106 \text{ H}_{2}\text{O}$$

$$\Rightarrow \text{Protoplasm} + 106 \text{ O}_{2} + 15\text{H}^{+}$$
(1-36a)

$$106 \text{ CO}_2 + 16 \text{ NO}_3^- + \text{H}_2\text{PO}_4^- + 122 \text{ H}_2\text{O} + 17\text{H} + \Rightarrow \text{Protoplasm} + 138 \text{ O}_2$$
 (1-36b)

The above equations present the stoichiometric description of the photosynthetic process assuming ammonium (Equation 1-36a) or nitrate (Equation 1-36b) as the nitrogen source and assuming algal biomass to have Redfield stoichiometry:



## TABLE 1-8. SILICA REACTION EQUATIONS

## Biogenic Silica (BSi)

$$S_{16} = \left(k_{_{PR}}(T) + k_{_{grz}}\left(T\right)\right) \cdot P_{_{c}} - k_{_{16,17}} \, \theta_{_{16,17}}^{\phantom{1}T-20} \cdot BSi \cdot \frac{P_{_{c}}}{K_{_{mP_{_{c}}}} + P_{_{c}}} - \frac{v_{_{s16}}}{H} \cdot BSi$$

### Available Silica (Si)

$$S_{17} = k_{16,17} \, \theta_{16,17}^{\quad T-20} \cdot BSi \cdot \frac{P_c}{K_{mP_c} + P_c} - \left(1 - f_{ExPP}^{}\right) \cdot a_{sc} \cdot G_P \cdot P_c$$

Murderkill River Model

Description	Notation	<u>Value</u>	<u>Units</u>
Phytoplankton Biomass	$P_c$	_	mgC/L
Temperature Corrected Algal Respiration Rate	$k_{PR}(T)$	Eq. 1-11a	day <sup>-1</sup>
Temperature Corrected Grazing Rate	$k_{grz}(T)$	Eq. 1-13	day-1
Specific Phytoplankton Growth Rate	$G_p$	Eq. 1-5	day-1
Silica to Carbon Ration	$a_{sc}$	Table 1-2	mgSi/mgC
Fraction of Primary Productivity Going to the Algal Exudate pool	$\mathrm{f_{ExPP}}$	0.1	
Mineralization Rate of Biogenic Silica	k <sub>16,17</sub>	0.1-0.25	day-1
Temperature Coefficient	$\boldsymbol{\theta}_{16,17}$	1.08	
Silica Settling Rate	$V_{s16}$	0.5-1.0	m/day



Biomass = 
$$C_{106} H_{263} O_{110} N_{16} P_1$$
 (1-37)

Oxygen-deficient or under-saturated waters are replenished via atmospheric reaeration. The reaeration coefficient is a function of the average tidal velocity, wind and temperature, and is computed using Equations 1-38a and 1-38b:

$$k_a (20^{\circ} C) = K_L / H$$
 wind (1-38a)

$$k_a(T) = k_a(20^{\circ}C)\theta_a^{T-20}$$
 temperature (1-38b)

where

 $k_a$  = the surface mass transfer coefficient (m/day),

H = depth (m),

 $\theta_a$  = temperature coefficient.

Dissolved oxygen saturation is a function of both temperature and salinity and is determined via Equation 1-39 (Standard Methods, 1992):

$$DO_{sat} = exp \left[ -139.34411 + 1.575701 \cdot 10^{5} / T -6.642308 \cdot 10^{7} / T^{2} + 1.243800 \cdot 10^{10} / T^{3} -8.621949 \cdot 10^{11} / T^{4} - S(1.7674 \cdot 10^{-2} -10.754 / T + 2140.7 / T^{2}) \right]$$

$$(1-39)$$

where

S = salinity (psu), T = temperature (°K).

Dissolved oxygen is diminished in the water column as a result of algal respiration, which is the reverse process of photosynthesis; as a result of nitrification:

$$NH_4^+ + 20_2 \Rightarrow NO_3^- + H_2O + 2H^+$$
 (1-40)



as a result of the oxidation of carbonaceous material (including detrital phytoplankton):

$$CH_2O + O_2 \Rightarrow CO_2 + H_2O \tag{1-41}$$

and, if dissolved oxygen concentrations are sufficiently low, as a result of denitrification:

$$5CH_2O + 4NO_3^- + \Rightarrow 5CO_2 + 2N_2 + 7H_2O$$
 (1-42)

Table 1-9 presents a summary of the dissolved oxygen mass balance equation and associated coefficients incorporated in the integrated eutrophication model.



## TABLE 1-9. DISSOLVED OXYGEN AND O<sup>\*</sup><sub>2</sub> REACTION RATES

## Sulfide Oxygen Equivalents (O<sub>2</sub>\*)

$$S_{24} = K_{O_{2}^{*}} \; \theta_{O_{2}^{*}}^{T-20} \cdot O_{2}^{*} \cdot \frac{P_{c}}{K_{mP_{c}} + P_{c}} \cdot \frac{DO}{K_{DO_{O_{c}^{*}}} + DO}$$

## Dissolved Oxygen (DO)

$$\begin{split} S_{25} &= a_{OC} \cdot \alpha_{NH_4} \cdot G_P \cdot P_c + \left(a_{NO_3}c\right) \cdot \left(1 - \alpha_{NH_4}\right) \cdot G_P \cdot P_c \\ &+ k_a \theta_a^{T-20} \cdot \left(DO_{sat} - DO\right) - a_{OC} \cdot k_{PR} \cdot (T) \cdot P_c \\ &- 2 \cdot a_{ON} \cdot k_{14,15} \theta_{14,15}^{T-20} \cdot NH_4 \cdot \frac{DO}{K_{nitr} + DO} \\ &- a_{OC} \cdot \left[k_{20,0} \, \theta_{20,0}^{T-20} \cdot RDOC + k_{21,0} \, \theta_{21,0}^{T-20} \cdot LDOC \cdot \frac{LDOC}{K_{m_{LDOC}} + LDOC} \right. \\ &+ k_{22,0} \, \theta_{22,0}^{T-20} \cdot Re \, DOC \cdot \frac{Re \, DOC}{K_{mLDOC} + Re \, DOC} \\ &+ k_{23,0} \, \theta_{23,0}^{T-20} \cdot ExDOC \cdot \frac{ExDOC}{K_{mLDOC} + ExDOC} \, \left] \cdot \frac{P_c}{K_{mPc} + P_c} \cdot \frac{DO}{K_{DO} + DO} \\ &- k_{\sigma_2^*} \theta_{\sigma_2^*}^{T-20} \cdot O_2^* \cdot \frac{P_c}{K_{mPc} + P_c} \cdot \frac{DO}{K_{DO_{\sigma_2^*}} + DO} \end{split}$$

TABLE 1-9. DISSO	LVED OXYGEN AND O2 REACTION RATES
	(continued)

Murderkill River Model

	minucu)			Model
Rate Constants				
Description	<u>Notation</u>	Value	<u>Units</u>	
Oxygen to Carbon Ratio	$a_{OC}$	32/12	$mgO_2/mg$ C	3.5
Oxygen to Nitrogen Ratio	$a_{ON}$	32/14	$mgO_2/mg\ N$	2.29
Oxygen to Carbon Ratio for Nitrate Uptake	$\alpha_{_{NO_3C}}$	$\frac{48}{14}$ a <sub>NC</sub>	$mgO_2/mg$ C	3.43
Reaeration Rate at 20°C	$k_a$	Eq. 1.19a	day <sup>-1</sup>	f(wind,vel)
Temperature Coefficient	$ heta_{ m a}$	1.024	none	1.024
Oxygen Transfer Coefficient	$k_{L}$	0.75-1.8	m/day	min 0.3
Dissolved Oxygen Saturation	$\mathrm{DO}_{\mathrm{sat}}$	Eq. 1.20	$\rm mgO_2/L$	
Oxidation Rates and Temperature Coefficients				
for RDOC	$\begin{matrix}\mathbf{k_{20,0}}\\\mathbf{\theta_{20,0}}\end{matrix}$	0.008-0.01 1.08	day <sup>-1</sup>	
for LDOC	$\begin{matrix}k_{21,0}\\\theta_{21,0}\end{matrix}$	0.10-0.15 1.047	day <sup>-1</sup>	
for ReDOC	$\begin{matrix}k_{22,0}\\\theta_{22,0}\end{matrix}$	0.25-0.3 1.047	day <sup>-1</sup>	
for ExDOC	$\begin{matrix}k_{23,0}\\\theta_{23,0}\end{matrix}$	0.1-0.125 1.08	day <sup>-1</sup>	
Oxidation Rate of Dissolved Sulfide	$k_{\mathfrak{o}_2^*}$	0.15-0.5	day <sup>-1</sup>	0.15
Temperature Coefficient	$\theta_{o_2^*}$	1.08		1.08
Half Saturation for Oxygen Limitation	$k_{{_{DO_{0_2^*}}}}$	0.2	${\rm mgO_2/L}$	0.1



### 1.2.4 Specification of Input Variables Associated with the Eutrophication Model

As described earlier, the user has the choice of two algal growth formulation - the standard formulation and the Laws-Chalup formulation. The user can also select whether to simulate one, two, or three algal groups. In addition, the user can select from various options to specify the reaeration coefficient and the extinction coefficient. These selections are provided for via the first three constants specified in Card Group L (more specifically in L10). These constants are described below.

Constant		
<u>Number</u>	<u>Name</u>	<u>Description</u>
1	AGOPT	algal growth model option
		= 0, use standard or traditional algal growth kinetics
		= 1, use Laws-Chalup formulation
2	ACTALG	number of algal groups to simulate
		= 1, just one group (state-variable #2) will be simulated
		= 2, two groups will be simulated (using state-variables #2 and #3)
		= 3, three algal groups will be simulated (using state-variables #2 through
		#4)
3	KAOPT	reaeration formulation option
		= 0, use spatially constant $k_L$ ( $k_a = k_L/depth$ )
		$=$ 1, use spatially variable $k_L$
		= 2, use velocity shear and oxygen diffusivity
		= 3, use wind shear formulation
4	KEOPT	extinction coefficient option
		= 0, k <sub>e</sub> is a constant (spatially and temporally invariant
		= 1, k <sub>e</sub> is a spatially variable but constant in time(using 2-d parameter
		array)
		= $2$ , $k_e$ is spatially invariant but varies in time (using time-variable
		function)
		= 3, k <sub>e</sub> is spatially variable and can vary in time, (using 2-d parameter
		array and one time-variable function)
		= 4, k <sub>e</sub> is spatially and temporally variable (requires separate input file)



# TABLE 1-10. KINETIC CONSTANTS USED FOR STANDARD EUTROPHICATION ALGAL GROWTH MODEL

If <AGOPT> = 0 then the following constants (9 through 99) are used by the eutrophication model and must be specified by the user. If the user is simulating only one phytoplankton group then constants 41-99 can be ignored; if the user is simulating two group then constants 73-99 can be ignored.

Number	<u>Name</u>	<u>Description</u>	<u>Units</u>
9	TOPT1	optimal growth temperature for algal group #1	deg C
10	K1BETA1	temperature correction effect on growth rate below <topt1></topt1>	(deg C) <sup>-2</sup>
11	K1BETA2	temperature correction effect on growth rate above <topt1></topt1>	(deg C) <sup>-2</sup>
12	K1C	saturated phytoplankton growth rate (at temperature = <topt1>)</topt1>	/day
13	K1T	temperature coefficient	
14	IS1	saturating algal light intensity	ly/day
15	KMN1	half saturation constant for nitrogen	mg N/L
16	KMP1	half saturation constant for phosphorous	mg P/L
17	KMS1	half saturation constant for silica	mg Si/L
18	K1RB	basal/resting respiration rate -or- endogenous respiration rate at 20 deg C	/day
19	K1RT	temperature coefficient	
20	K1RG	growth-rate-dependent respiration coefficient	
21	K1GRZC	death rate due to grazing	/day
22	K1GRZT	temperature coefficient	
23	CCHL1	carbon to chlorophyll ratio	mg C/mg Chla
24	CRBP11	carbon to phosphorus ratio - non-P limited	mg C/mg P
25	CRBP12	carbon to phosphorus ratio - P limited	mg C/mg P
26	CRBP13	coefficient determining range of P limitation	L/mg P
27	CRBN11	carbon to nitrogen ratio - non-N limited	mg C/mg N
28	CRBN12	carbon to nitrogen ratio - N limited	mg C/mg N
29	CRBN13	coefficient determining range of N limitation	L/mg N
30	CRBS11	carbon to silica ratio - non-Si limited	mg C/mg Si
31	CRBS12	carbon to silica ratio - Si limited	mg C/mg Si
32	CRBS13	coefficient determining range of Si limitation	L/mg Si
33	XKC1	chlorophyll self-shading extinction coefficient	m²/mg Chla
34	VSBAS1	base algal settling rate	m/day
35	VSNTR1	nutrient stressed algal settling rate	m/day



# TABLE 1-10. KINETIC CONSTANTS USED FOR STANDARD EUTROPHICATION ALGAL GROWTH MODEL (Continued)

41	TOPT2	optimal growth temperature for algal group #2	deg C
42	K2BETA1	temperature correction effect on growth rate below <topt2></topt2>	$(\deg C)^{-2}$
43	K2BETA2	temperature correction effect on growth rate above <topt2></topt2>	(deg C) <sup>-2</sup>
44	K2C	saturated phytoplankton growth rate (at temperature = <topt2>)</topt2>	/day
45	K2T	temperature coefficient	
46	IS2	saturating algal light intensity	ly/day
47	KMN2	half saturation constant for nitrogen	mg N/L
48	KMP2	half saturation constant for phosphorous	mg P/L
49	KMS2	half saturation constant for silica	mg Si/L
50	K2RB	basal/resting respiration rate -or-	/day
		endogenous respiration rate at 20 deg C	/day
51	K2RT	temperature coefficient	·
52	K2RG	growth-rate-dependent respiration coefficient	
53	K2GRZC	death rate due to grazing	/day
54	K2GRZT	temperature coefficient	·
55	CCHL2	carbon to chlorophyll ratio	mg C/mg Chla
56	CRBP21	carbon to phosphorus ratio - non-P limited	mg C/mg P
57	CRBP22	carbon to phosphorus ratio - P limited	mg C/mg P
58	CRBP23	coefficient determining range of P limitation	L/mg P
59	CRBN21	carbon to nitrogen ratio - non-N limited	mg C/mg N
60	CRBN22	carbon to nitrogen ratio - N limited	mg C/mg N
61	CRBN23	coefficient determining range of N limitation	L/mg N
62	CRBS21	carbon to silica ratio - non-Si limited	mg C/mg Si
63	CRBS22	carbon to silica ratio - Si limited	mg C/mg Si
64	CRBS23	coefficient determining range of Si limitation	L/mg Si
65	XKC2	chlorophyll self-shading extinction coefficient	m²/mg Chla
66	VSBAS2	base algal settling rate	m/day
67	VSNTR2	nutrient stressed algal settling rate	m/day



TABLE 1-10. KINETIC CONSTANTS USED FOR STANDARD EUTROPHICATION ALGAL GROWTH MODEL (Continued)

73	TOPT3	optimal growth temperature for algal group #3	deg C
74	K3BETA1	temperature correction effect on growth	$(\deg C)^{-2}$
		rate below <topt1></topt1>	(338 3)
75	K3BETA2	temperature correction effect on growth	(deg C) <sup>-2</sup>
		rate above <topt1></topt1>	(338 3)
76	K3C	saturated phytoplankton growth rate	/day
, 0	1100	(at temperature = <topt1>)</topt1>	, day
77	К3Т	temperature coefficient	
78	IS3	saturating algal light intensity	ly/day
79	KMN3	half saturation constant for nitrogen	mg N/L
80	KMP3	half saturation constant for phosphorous	mg P/L
81	KMS3	half saturation constant for silica	mg Si/L
82	K1RB	basal/resting respiration rate -or-	/day
<b>02</b>	TTTE	endogenous respiration rate at 20 deg C	/day
83	K3RT	temperature coefficient	, day
84	K3RG	growth-rate-dependent respiration coefficient	
85	K3GRZC	death rate due to grazing	/day
86	K3GRZT	temperature coefficient	, day
87	CCHL3	carbon to chlorophyll ratio	mg C/mg Chla
88	CRBP31	carbon to phosphorus ratio - non-P limited	mg C/mg P
89	CRBP32	carbon to phosphorus ratio - P limited	mg C/mg P
90	CRBP33	coefficient determining range of P limitation	L/mg P
91	CRBN31	carbon to nitrogen ratio - non-N limited	mg C/mg N
92	CRBN32	carbon to nitrogen ratio - N limited	mg C/mg N
93	CRBN33	coefficient determining range of N limitation	L/mg N
94	CRBS31	carbon to silica ratio - non-Si limited	mg C/mg Si
95	CRBS32	carbon to silica ratio - Si limited	mg C/mg Si
96	CRBS33	coefficient determining range of Si limitation	L/mg Si
97	XKC3	chlorophyll self-shading extinction coefficient	m²/mg Chla
98	VSBAS3	base algal settling rate	m/day
99	VSNTR3	nutrient stressed algal settling rate	m/day
105	KMPHYT	half saturation constant for phytoplankton	mg C/L
		1 / 1	0 /



## TABLE 1-11. KINETIC CONSTANTS USED FOR LAWS-CHALUP EUTROPHICATION ALGAL GROWTH MODEL

If <AGOPT> = 1 then the following constants (6 through 95) are used by the eutrophication model and must be specified by the user. If the user is simulating only one phytoplankton group, then constants 41-95 can be ignored; if the user is simulating only two groups, then constants 73-95 can be ignored.

9	TOPT1	optimal growth temperature for algal group #1	deg C
10	K1BETA1	temperature correction effect on growth rate below <topt1></topt1>	(deg C) <sup>-2</sup>
11	K1BETA2	temperature correction effect on growth rate above <topt1></topt1>	(deg C) <sup>-2</sup>
12	GPRE1	gross photosynthetic rate per unit cell (associated with photosynthetic dark reactions)	/day
13	GPR01	gross photosynthetic rate per unit cell per unit light intensity under nutrient-saturated conditions and zero irradiance	m <sup>2</sup> /mol quanta
14	IS1	saturating algal light intensity	ly/day
15	KMN1	half saturation constant for nitrogen	mg N/L
16	KMP1	half saturation constant for phosphorous	mg P/L
17	KMS1	half saturation constant for silica	mg Si/L
18	K1RB	basal or resting respiration rate	/day
19	K1RT	temperature coefficient for basal/endogenous respiration	•
20	K1RG	growth-rate-dependent respiration coefficient	
21	K1GRZC	death rate due to grazing	/day
22	K1GRZT	temperature coefficient	·
23	FSC1	fraction of C allocated to structural purposes	
24	WCCHL1	carbon to chlorophyll ratio	mg C/mg Chla
25	WCP1	carbon to phosphorus ratio - non-P limited	mg C/mg P
26	WCN1	carbon to nitrogen ratio - non-N limited	mg C/mg N
27	WCS1	carbon to silica ratio - non-Si limited	mg C/mg Si
28	QF1	quotient of nutrient-limited nutrient:C ratios	
		at relative growth rates of 0 and 1	
29	XKC1	chlorophyll self-shading extinction coefficient	m²/mg Chla
30	VSBAS1	base algal settling rate	m/day
31	VSNTR1	nutrient stressed algal settling rate	m/day



# TABLE 1-11. KINETIC CONSTANTS USED FOR LAWS-CHALUP EUTROPHICATION ALGAL GROWTH MODEL (Continued)

41	TOPT2	optimal growth temperature for algal group #2	deg C
42	K2BETA1	temperature correction effect on growth rate	$(\deg C)^{-2}$
		below <topt2></topt2>	
43	K2BETA2	temperature correction effect on growth rate	(deg C) <sup>-2</sup>
		above <topt2></topt2>	
44	GPRE2	gross photosynthetic rate per unit cell (associated	/day
		with photosynthetic dark reactions)	
45	GPR02	gross photosynthetic rate per unit cell per unit	m²/mol quanta
		light intensity under nutrient-saturated conditions	
		and zero irradiance	
46	IS2	saturating algal light intensity	ly/day
47	KMN2	half saturation constant for nitrogen	mg N/L
48	KMP2	half saturation constant for phosphorous	mg P/L
49	KMS2	half saturation constant for silica	mg Si/L
50	K2RB	basal or resting respiration rate	/day
51	K2RT	temperature coefficient for basal/endogenous respiration	
52	K2RG	growth-rate-dependent respiration coefficient	
53	K2GRZC	death rate due to grazing	/day
54	K2GRZT	temperature coefficient	
55	FSC2	fraction of C allocated to structural purposes	
56	WCCHL2	carbon to chlorophyll ratio	mg C/mg Chla
57	WCP2	carbon to phosphorus ratio - non-P limited	mg C/mg P
58	WCN2	carbon to nitrogen ratio - non-N limited	mg C/mg N
59	WCS2	carbon to silica ratio - non-Si limited	mg C/mg Si
60	QF2	quotient of nutrient-limited nutrient: C ratios at relative	
		growth rates of 0 and 1	
61	XKC2	chlorophyll self-shading extinction coefficient	m²/mg Chla
62	VSBAS2	base algal settling rate	m/day
63	VSNTR2	nutrient stressed algal settling rate	m/day



# TABLE 1-11. KINETIC CONSTANTS USED FOR LAWS-CHALUP EUTROPHICATION ALGAL GROWTH MODEL (Continued)

73	TOPT3	optimal growth temperature for algal group #3	deg C
74	K3BETA1	temperature correction effect on growth rate	(deg C) <sup>-2</sup>
7.	IZADETE A A	below <topt1></topt1>	(1 0)-2
75	K3BETA2	temperature correction effect on growth rate above <topt1></topt1>	(deg C) <sup>-2</sup>
76	GPRE3	gross photosynthetic rate per unit cell (associated	/day
		with photosynthetic dark reactions)	2.4
77	GPR03	gross photosynthetic rate per unit cell per unit	m²/mol quanta
		light intensity under nutrient-saturated conditions	
		and zero irradiance	
78	IS3	saturating algal light intensity	ly/day
79	KMN3	half saturation constant for nitrogen	mg N/L
80	KMP3	half saturation constant for phosphorous	mg P/L
81	KMS3	half saturation constant for silica	mg Si/L
82	K3RB	basal or resting respiration rate	/day
83	K3RT	temperature coefficient for basal/endogenous	
84	K3RG	growth-rate-dependent respiration coefficient	
		respiration	
85	K3GRZC	death rate due to grazing	/day
86	K3GRZT	temperature coefficient	·
87	FSC3	fraction of C allocated to structural purposes	
88	WCCHL3	carbon to chlorophyll ratio	mg C/mg Chla
89	WCP3	carbon to phosphorus ratio - non-P limited	mg C/mg P
90	WCN3	carbon to nitrogen ratio - non-N limited	mg C/mg N
91	WCS3	carbon to silica ratio - non-Si limited	mg C/mg Si
92	QF3	quotient of nutrient-limited nutrient: C ratios	
	-	at relative growth rates of 0 and 1	
93	XKC3	chlorophyll self-shading extinction coefficient	m <sup>2</sup> /mg Chla
94	VSBAS3	base algal settling rate	m/day
95	VSNWTR3	nutrient stressed algal settling rate	m/day
105	KMPHYT	half saturation constant for phytoplankton	mg C/L
	<del>-</del>	r yer	0 -1 -



## TABLE 1-12. REMAINING KINETIC CONSTANTS USED FOR INTEGRATED EUTROPHICATION MODEL

		Recycle Fractions - Fraction of Grayed/Respired Algal Biomass Going	r to
106	FRPOP	refractory particulate organic phosphorous	5 10
107	FLPOP	labile particulate organic phosphorous	
108	FRDOP	refractory dissolved organic phosphorous	
109	FLDOP	labile dissolved organic phosphorous	
110	FPO4	dissolved inorganic phosphorous	
111	FRPON	refractory particulate organic nitrogen	
112	FLPON	labile particulate organic nitrogen	
113	FRDON	refractory dissolved organic nitrogen	
114	FLDON	labile dissolved organic nitrogen	
115	FNH4	ammonia	
116	FRPOC	refractory particulate organic carbon	
117	FLPOC	labile particulate organic carbon	
118	FRDOC	refractory dissolved organic carbon	
119	FLDOC	labile dissolved organic carbon	
		Phosphorus Hydrolysis/Mineralization Rates at 20 deg C	
120	K57C	hydrolysis rate of RPOP to RDOP	/day
121	K57T	temperature coefficient	
122	K68C	hydrolysis rate of LPOP to LDOP	/day
123	K68T	temperature coefficient	
124	K79C	mineralization rate of RDOP to PO4	/day
125	K79T	temperature coefficient	
126	K89C	mineralization rate of LDOP to PO4	/day
127	K89T	temperature coefficient	
		Nitrogen Hydrolysis/Mineralization Rates at 20 deg C	
128	K1012C	hydrolysis rate of RPON to RDON	/day
129	K1012T	temperature coefficient	
130	K1113C	hydrolysis rate of LPON to LDON	/day
131	K1113T	temperature coefficient	
132	K1214C	mineralization rate of RDON to NH4	/day
133	K1214T	temperature coefficient	
134	K1314C	mineralization rate of LDON to NH4	/day
135	K1314T	temperature coefficient	



# TABLE 1-12. REMAINING KINETIC CONSTANTS USED FOR INTEGRATED EUTROPHICATION MODEL (Continued)

		Nitrification/Denitification Rates	
136		nitrification rate at 20 deg C	/day
137		temperature coefficient	
138		half saturation constant for nitrification oxygen limitation	mg $\mathrm{O}2/\mathrm{L}$
139		denitrification rate at 20 deg C	/day
140		temperature coefficient	
141	KNO3	Michaelis constant for denitrification oxygen limitation	mg O2/L
		Silica Mineralization Rates at 20 deg C	
142	K1617C	mineralization rate of biogenic Si to available dissolved Si	/day
143	K1617T	temperature coefficient	,,
		Carbon Hydrolysis/Oxidation Rates at 20 deg C	
144		hydrolysis rate of RPOC to RDOC	/day
145		temperature coefficient	
146		hydrolysis rate of LPOC to LDOC	/day
147		temperature coefficient	
148	K200C	oxidation rate of RDOC	/day
149		temperature coefficient	
150		oxidation rate of LDOC	/day
151	K210T	temperature coefficient	
152		Michaelis constant for LDOC	mg C/L
153	KDOC	half saturation constant for organic carbon	mg $\mathrm{O}2/\mathrm{L}$
154		algal exudate DOC oxidation rate	/day
155	K220T	temperature coefficient	
156	FLOCEX	fraction of primary productivity going to labile organic	
		carbon via exudation	
157	K2324C	hydrolysis rate of REPOC to REDOC	/day
158	K2324T	temperature coefficient	
159	K240C	reactive DOC oxidation rate	/day
160	K240T	temperature coefficient	
161	CTOPCSO	carbon to phosphorus ratio of CSO solids	mg C/mg P
162	CTONCSO	carbon to nitrogen ratio of CSO solids	mg C/mg N
163	K250C	oxidation rate for aqueous sod	/day
164	K250T	temperature coefficient	,,
		1	



# TABLE 1-12. REMAINING KINETIC CONSTANTS USED FOR INTEGRATED EUTROPHICATION MODEL (Continued)

165	KO2EQ	half saturation constant for $O_2^*$	${ m mg~O_2/L}$
166	KLMIN	if $\langle KAOPT \rangle = 0$ , then $K_{lmin} = K_{l}$	m/day
		if $\langle KAOPT \rangle > 0$ , then $K_{lmin} = minimum$ value for $K_{l}$	•
167	DIFUS	diffusivity of oxygen across the air-water interface	m²/day
168	KAT	temperature correction coefficient for atmospheric reaeration	-
169	VSBAST	temperature correction	
170	VSPOM	particulate organic matter settling rate	m/day
171	VSPMT	temperature correction	
172	VSSEDT	temperature correction for deposition to sediment	
173	BVCSO	power coefficient for CSO solid settling rate (>=1)	unitless
174	CRCSO	critical REPOC concentration for CSO settling function	mg C/L
175	VMINCSO	minimum settling rate for CSO solids	m/day
		Vcso =min (VMAXCSO + VMINCSO + (VMAXCSO - VMINC	CSO)
		* (REPOC/CRCSO)**BVCSO)	
176	VMAXCSO	maximum settling rate for CSO solids	m/day
177	KADPO4	partition coefficient for sorbed phosphorus	L/mg ss
178	KADSI	partition coefficient for sorbed silica	L/mg ss
179	VSPIM	settling rate for phosphorus/silica sorbed to suspended	m/day
		solids	
180	KECONST	base (chl-a corrected) extinction coefficient (used when	/m
		$\langle KEOPT \rangle = 0.2$	



### 1.2.4.1 Parameters, Constants, and Time Functions

The parameters, constants, and time functions required by the kinetics of this model are specified according to the formatting described for input Group L in the RCA Users Guide. Table 1-13 lists the required two dimensional segment parameters. No three dimensional parameters are included in the kinetic routine. Required time variable functions are described in Table 1-14.

Number	Name	Description	Units
1	KL	transfer coefficient for reaeration	m/day
2	VSNET1	settling efficiency from water column to the bed for algal group number 1 (the winter diatom group)	
3	VSNET2	settling efficiency from water column to the bed for algal group number 2 (the summer mixed assemblage)	m/day
4	VSNET3	settling efficiency from water column to bed for algal group number 3	m/day
5	VSNET4	settling efficiency from water column to the bed for non-living particulate organic matter (POM)	m/day
6	KEBS	base extinction coefficient (when KEOPT - 1 or 3)	m <sup>-1</sup>

TABLE 1-13. 2-D PARAMETERS

Note: by settling efficiency, it is meant the "stickiness" of a particle settling from the water column to the sediment bed; range 0 to 1. If VSNET = 1, all of the particles settling from the water column to the bed, stick to the bed and become incorporated in the sediment. If VSNET = 0.5, only half of the particles settling from the water column to the bed become incorporated in the sediment; the remainder are assumed to become "resuspended" and may be transported elsewhere. If VSNET = 0, none of the particles settle to the bed, i.e., no deposition in this segment.

Number	Name	Description	Units
1	ITOTSF	total daily solar radiation	ly/day
2	F	fraction of daylight	day
3	WIND	wind speed	m/sec
4	KETVF	extinction coefficient (when KEOPT = 2 or 3)	m <sup>-1</sup>

TABLE 1-14. TIME-VARIABLE FUNCTIONS

Table 1-15 presents a sample input deck for the standard eutrophication model coefficient set, which includes one kinetic subroutine specific file, i.e., the sediment nutrient flux subroutine input data set.

TABLE C N2DP	ARAM	SAMPLE	EUTROPHICATIO	N INPUT	DATASET			
	6 ale1 3048	Scale2		Scale4				
0.	0000 0000 0000	0.0000 0.7870 0.0000	0.0000					
0.	- alga 0000 0000 0000	al group 0.0000 1.0000 0.0000	0.0000					
0.	- alga 0000 0000 0000	al group 0.0000 1.0000 0.0000	0.0000					
Vsnet3 0. 0.		al group 0.0000 1.0000 0.0000	0.0000					
0. 0.	- pom 0000 0000 0000	0.0000 1.0000 0.0000	0.0000					
0.	0000 0000 0000	0.0000	0.0000					
	CARAM CALE1 DE-20				number of	3D paramet	cers	
	7/L) 0.01 0.01 0.01 0.01 0.01	0.01 0.01 0.01 0.01 0.01	0.01 0.01 0.01 0.01		Layer #1			
C N	0.01 ICONS	0.01	0.01		Layer #2	_		
A	180 GOPT	ACTALG		KEOPT	numbe Unused	er of consta d Unused	unts Unused	Unused
C	0. COPT1 3.50 KMS1 0.020 CPR12 0.0 XKC1	2. K1BETA1 .004 K1RE 0.075 CPR13 0.0 VSBAS1	K2BETA2 .006 K1RT 1.047 CNR11 5.670 VSNTR1	2. K1C 2.500 K1RG 0.0 CNR12 0.0 Unused	K1T 1.068 K1GZC 0.100 CNR13 0.0	3 150.000 K1GZT 1.10 CSR11 5.0	KMN1 0.010 CCHL1 30.0 CSR12 10.0 Unused	KMP1 0.001 CPR11 40.0 CSR13 0.0 Unused
T 0 0	COPT2 22. KMS2 0.002 CPR22 0.0 XKC2	0.2 K2BETA1 .004 K2RE 0.075 CPR23 0.0 VSBAS2	K2BETA2 .006 K2RT 1.047 CNR21 5.670 VSNTR2	K2C 2.400 K2RG 0.0 CNR22 0.0 Unused	K2T 1.068 K2GZC 0.120 CNR23 0.0 Unused	350.0 K2GRT 1.100 CSR21 8.0	KMN2 0.010 CCHL2 80.0 CSR22 0.0 Unused	KMP2 0.001 CPR21 40.0 CSR23 0.0 Unused
Ι	0.017 OPT3 0. KMS3 0. CPR32	0.5 K3BETA1 0. K3RE 0. CPR33	K3BETA2 0. 8 K3RT 0.	K3C 0. K3RG 0. CNR32	K3T 0. K3GZC 0. CNR33	0. C K3GRT 0.	KMN3 0. CCHL3 0. CSR32	KMP3 0. CPR31 0. CSR33



TAB	LE 1-15.		EUTROPHICAT					•
	0. XKC3	0. VSBAS3	0. VSNTR3	0. Unused	0. Unused	0. Unused	0. Unused	0. Unused
	0. KMPHY 0.050 FRDON 0.125 K57T 1.080 K1012T 1.080 K1415T 1.040 K1820T 1.080 KDOC 0.200 CTOPCSO 35. VSBAST 1.000 VSPIM	0. FRPOP 0.100 FLDON 0.125 K68C 0.070 K1113C 0.050 KNIT 1.500 K1921C 0.070 K220C 0.120 CTONCSO 6.0 VSPOM 0.750	0. FLPOP 0.250 FNH4 0.350 K68T 1.080 K1113T 1.080 K150C 0.050 K1921T 1.080 K220T 1.047 K250C 0.150 VSPMT 1.00	FRDOP 0.100 FRPOC 0.001 K79C 0.020 K1214C 0.010 K150T 1.045 K200C 0.010 FLOCEX 0.0 K250T 1.080 VSSEDT 1.0	FLDOP 0.100 FLPOC 0.449 K79T 1.080 K1214T 1.080 KNO3 0.010 K200T 1.080 K2324C 0.35 K02EQ 0.100 BVCSO 2.0	FPO4 0.450 FRDOC 0.100 K89C 0.090 K1314C 0.075 K1617C 0.10 K210C 0.150 K2324T 1.047 KLMIN 2.0 CRCSO 10.	FRPON 0.001 FLDOC 0.450 K89T 1.080 K1314T 1.080 K1617T 1.080 K210T 1.047 K240C 0.100 DIFUS 0.00 KADPO4 6.0	FLPON 0.399 K57C 0.010 K1012C 0.010 K1415C 0.040 K1820C 0.010 KMLDOC 0.100 K24OT 1.080 KAT 1.024 KADSI 6.0
С	0.0 NOTVF	KECONST 0.0 TVPWLOPT 1		numbo	er of time	functions		
С	PNAME	NOBRK	TWARPTVF	nullibe	i or time	Tunctions		
_	ITOT	13	DAYS	TOTAL	DAILY RAD			
	118. 418. 418.	0. 120. 243.	168. 468. 318.	11. 151. 273.	218. 518. 218.	59. 181. 304.	318. 468. 168.	90. 212. 335.
С	118. PNAME F DAY 0.37 0.58	365. NOBRK 13 0. 120.	TWARPTVF DAYS 0.42 0.61	FRACT 31. 151.	TION OF DAY 0.46 0.63	LIGHT 59. 181.	0.52 0.59	90. 212.
	0.54	243.	0.49	273.	0.43	304.	0.40	335.
C C	0.37 PNAME Wind 000. PNAME	365. NOBRK 2 0. NOBRK	TWARPTVF DAYS 000. TWARPTVF	Wind 9999.	Speed (m/s	ec)		
C	KE	13	DAYS	Extin	ction coef	ficient (/	m)	
	0.70 0.73 0.57 0.67	0. 120. 243. 365.	0.65 0.96 0.57	31. 151. 273.	0.60 1.12 0.51	59. 181. 304.	0.55 0.74 0.63	90. 212. 335.
C N	OKINFIL 1			Numbe	r of kinet	ic subrout	ine specif	ic files
sed	.inp							





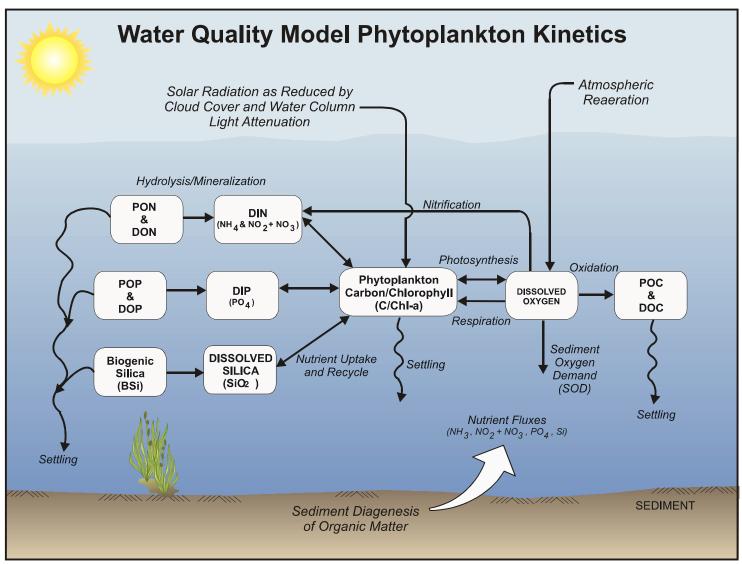


Figure 1-1. Principal Kinetic Interactions for Nutrient Cycles and Dissolved Oxygen



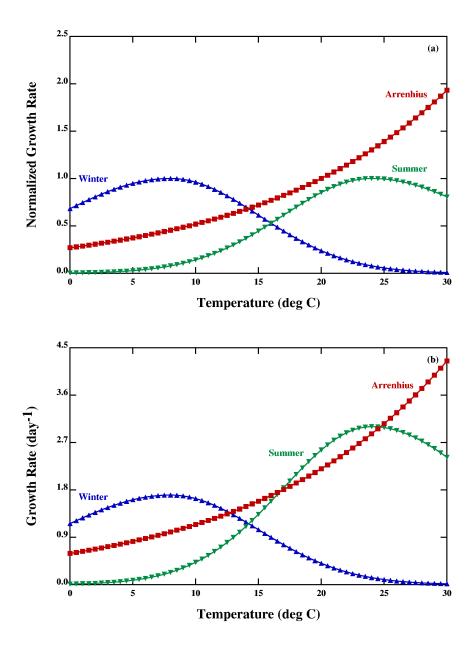


Figure 1-2. Growth Rate as a Function of Temperature



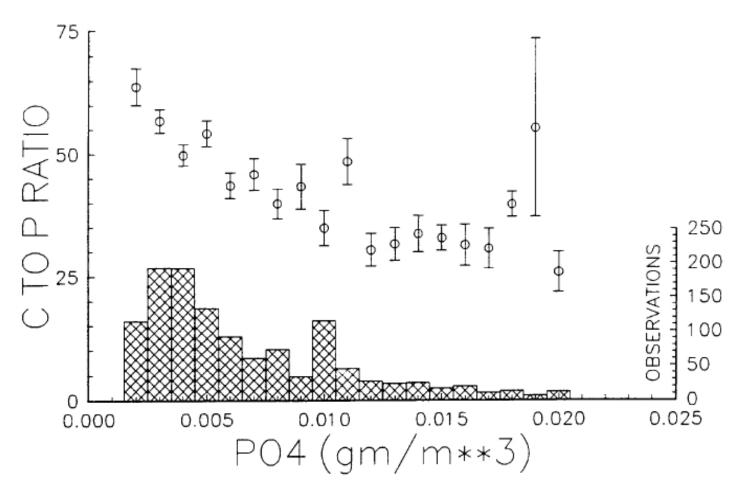


Figure 1-3. Carbon-to-phosphorus ratio (mean and standard error) of seston in Upper Chesapeake Bay. Bars show number of observations.



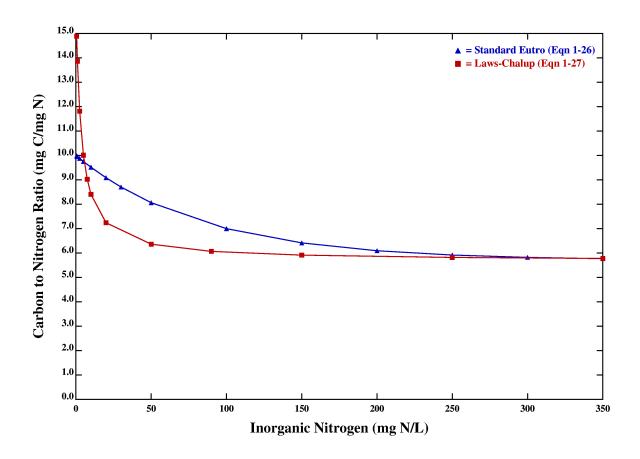
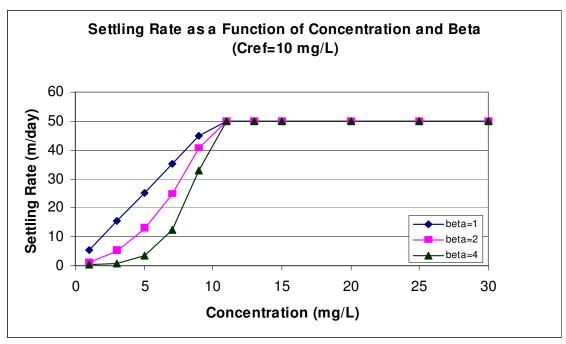


Figure 1-4. Carbon to nitrogen ratios as a function of the concentration of dissolved inorganic nitrogen.





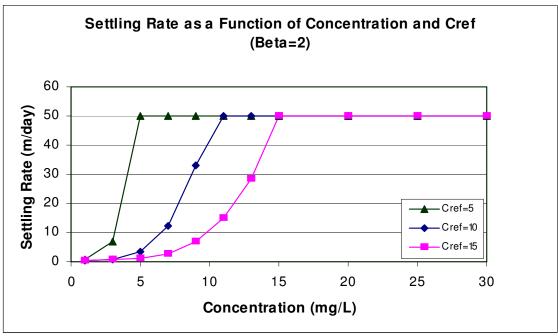


Figure 1-5. Settling Rate as a Function of Concentration and  $\beta$  (Beta) and  $C_{ref}$ 



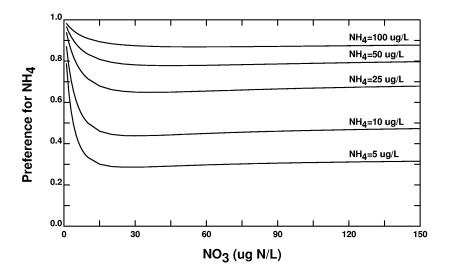


Figure 1-6. Behavior of the Ammonia Preference Structure for Various Concentrations of  $NH_3$  and  $NO_2+NO_3$ .



#### 2.0 FRAMEWORK FOR THE SEDIMENT FLUX SUBMODEL

#### 2.1 Overview of Model Framework

The sediment receives fluxes of particulate organic carbon (POC), particulate organic nitrogen (PON), and particulate organic phosphorus (POP). This is collectively referred to as particulate organic matter (POM). Mineralization, which is termed diagenesis, produces soluble end-products. These can react in the aerobic and anaerobic layers of the sediment. The difference between the resulting aerobic layer dissolved concentration and the overlying water concentration determines the flux to or from the sediment. The magnitude of the flux is determined by the surface mass transfer coefficient.

#### 2.2 Diagenesis

The water column model state-variables that are deposited to the sediment include: detrital algae, labile and refractory POC, labile and refractory PON, and labile and refractory POP. The fluxes of these state variables make up the incoming sources of particulate organic matter to the sediment. Carbon, nitrogen, and phosphorus are treated analogously.

The multi-class G model (Westrich and Berner 1984) is used as the basis for the diagenesis of POM. Each class represents a portion of the organic material that reacts at a specific rate. The reaction rates for each class are approximately an order of magnitude smaller than the previous class. For this application three G classes are chosen. The three classes represent three scales of reactivity: reactive (~20 day half life); refractory (~1 year half life); and inert (i.e., conservative). Particulate organic matter is also allowed to be removed by burial.

The kinetic equations for particulate organic carbon, nitrogen, and phosphorus are analogous. Let  $G_{POC,i}$  be the concentration of POC in the i<sup>th</sup> diagenesis class (i=1, 2, or 3). The kinetic equation for diagenesis is:

$$H\frac{dG_{POC,i}}{dt} = -k_{GPOC,i} \theta_{GPOC,i}^{T-20} G_{POC,i} H + J_{GPOC,i}(t)$$
(2-1)

where:

H = depth of the active sediment layer [m],

 $G_{POCi}$  = concentration of particulate organic carbon in reactivity class i,  $(g/m^3)$ 

 $k_{GPOC,i}$  = first order reaction rate coefficient ( $k_{GPOC,3} = 0$ ), (/day),



 $\theta_{GPOC,i}$  = temperature coefficient,  $J_{GPOC,i}(t)$  = POC flux of the i<sup>th</sup> G class to the sediment from the overlying water, (g/m²-day).

The water column sources that contribute to each reactivity class are:

 $J_{GPOC,1} = f_{G1} J_{POC}$   $J_{GPOC,2} = f_{G2} J_{POC}$  $J_{GPOC,3} = f_{G3} J_{POC}$ 

where:

 $f_{G1}$  = fraction of water column POC that is in reactivity class  $G_1$   $f_{G2}$  = fraction of water column POC that is in reactivity class  $G_2$  $f_{G3}$  = fraction of water column POC that is in reactivity class  $G_3$ 

 $J_{POC}$  = total flux of POC from the overlying water column to the sediment bed

Carbon diagenesis flux,  $J_C$ , is computed from the rates of mineralization of the labile and refractory G classes. (Note: it is assumed that  $G_3$  carbon is inert; therefore, it does not contribute to carbon diagenesis):

$$J_{C} = \sum_{i=1}^{2} k_{GPOC,i} \; \theta_{GPOC,i}^{(T-20)} \; G_{POC,i} \; H$$
 (2-2)

Nitrogen and phosphorus are completely analogous.

$$J_{N} = \sum_{i=1}^{2} k_{GPON,i} \theta_{GPON,i}^{(T-20)} G_{PON,i} H$$
 (2-3)

$$J_{P} = \sum_{i=1}^{2} k_{GPOP,i} \theta_{GPOP,i}^{(T-20)} G_{POP,i} H$$
 (2-4)

The reaction rates and temperature coefficients are analogous to those listed above for carbon.



### 2.3 The General Sediment Model Equations

The sediment model is constructed from a mass balance equation in the aerobic layer, denoted as layer 1, and the anaerobic layer, layer 2 (with the overlying water column concentrations denoted using the subscript 0). The equations are expressed in terms of the total concentration of the chemical. The distribution between particulate and dissolved fractions is modeled using a linear partitioning model. The mass balance equations of the model can be expressed in a general form which is quite convenient for numerical solution. The layer 1 and 2 equations are:

$$H_{1} \frac{dC_{T1}}{dt} = K_{L01} (f_{d1}C_{T1} - C_{d0}) + w_{12} (f_{p2}C_{T2} - f_{p1}C_{T1}) + K_{L12} (f_{d2}C_{T2} - f_{d1}C_{T1}) - k_{1}H_{1}C_{T1} + J_{T1}$$
(2-5)

$$H_{2} \frac{dC_{T2}}{dt} = -w_{12} (f_{p2}C_{T2} - f_{p1}C_{T1}) - K_{L12} (f_{d2}C_{T2} - f_{d1}C) - k_{2} H_{2} C_{T2} - w_{2}C_{T2} + J_{T2}$$
(2-6)

where:

 $C_{T1}$  = total concentration in layer 1 [M/L<sup>3</sup>],  $C_{T2}$  = total concentration in layer 2 [M/L<sup>3</sup>],  $f_{d1}$  = dissolved fraction in layer 1,  $\frac{1}{1 + m_2 \pi_2}$ 

 $f_{p1} = 1 - f_{d1} = particulate fraction in layer 1,$ 

 $f_{d2} = \frac{1}{1 + m_2 \pi_2}$  dissolved fraction in layer 2,

 $C_{p2}$  =  $f_{p2} C_{T2}$  = particulate concentration in layer 2 [M/L<sup>3</sup>],

 $C_{d0}$  = dissolved concentration,

 $J_{T1}$  = total source into layer 1 [M/L<sup>2</sup>-T],  $J_{T2}$  = total source into layer 2 [M/L<sup>2</sup>-T],

 $H_1$  = depth of layer 1 [L],  $H_2$  = depth of layer 2 [L],

 $K_{L01}$  = aqueous mass transfer coefficient between layer 1 and the overlying water [L/T],

 $K_{L12}$  = aqueous mass transfer coefficient between layer 1 and layer 2 [L/T],

 $w_{12}$  = particle mixing velocity between layer 1 and layer 2 [L/T],

 $w_2$  = sedimentation velocity out of layer 2 [L/T],



k<sub>1</sub> = first order decay rate coefficient removal process in layer 1 [T<sup>-1</sup>],
 k<sub>2</sub> = first order decay rate coefficient removal process in layer 2 [T<sup>-1</sup>].

The dissolved and particulate concentrations and fractions are:

 $C_{d1} = f_{d1}C_{T1} = dissolved concentration in layer 1 [M/L<sup>3</sup>],$ 

$$f_{_{d1}}=\frac{1}{1\!+\!m_{_{1}}\pi_{_{1}}}$$

 $C_{p1} = f_{p1} C_{T1} = particulate concentrations in layer 1 [M/L<sup>3</sup>],$ 

 $C_{d2}$  =  $f_{d2} C_{T2}$  = dissolved fraction in layer 2 [M/L<sup>3</sup>],

 $f_{p2}$  = 1 -  $f_{d2}$  = particulate fraction in layer 2,

where:

 $m_1$  = solids concentration in layer 1 (aerobic layer) [M/L<sup>3</sup>],  $m_2$  = solids concentration in layer 2 (anerobic layer) [M/L<sup>3</sup>],

 $\pi_1$  = partition coefficient in layer 1 [L<sup>3</sup>/M],  $\pi_2$  = partition coefficient in layer 2 [L<sup>3</sup>/M].

#### 2.3.1 Surface Mass Transfer Coefficient and Reaction Velocities

The surface mass transfer coefficient,  $K_{L01}$ , quantifies the mixing between layer 1 and the overlying water. The critical observation is that it can be related to the sediment oxygen demand, SOD. The SOD is the mass flux of dissolved oxygen into the sediment. Thus, it can be calculated from the mass transfer equation:

$$D_{1} \frac{d[O_{2}]}{dz}\Big|_{z=0} \approx D_{1} \frac{[O_{2}(0)] - [O_{2}(H_{1})]}{H_{1}} = \frac{D_{1}}{H_{1}} [O_{2}(0)]$$
(2-7)

where a straight line approximation to the derivative is used. The second equality follows from  $[O_2(H_1)] = 0$ , since  $H_1$  is the depth of zero oxygen concentration. Therefore, the surface mass transfer coefficient can be expressed as:



$$K_{L01} = \frac{D_1}{H_1} = \frac{SOD}{[O_2(0)]} = s$$
 (2-8)

which is the ratio of SOD and overlying water oxygen concentration. For notational simplicity this ratio is termed s.

The reaction rate in the aerobic layer is formulated as a conventional first order reaction with reaction rate constant  $k_1$ . The term in the layer 1 equation is  $k_1H_1$ . The depth of the aerobic zone follows from the definition of the surface mass transfer coefficient:  $s = D_1/H_1$ . Hence  $k_1H_1 = k_1D_1/s$ . The reaction velocity, which has units [L/T], is defined as:

$$\kappa_1 = \sqrt{D_1 k_1} \tag{2-9}$$

The square root is used to conform to the parameter group that appears in the spatially continuous form of the model. With these definitions the reaction rate - aerobic layer depth product becomes:

$$K_1 H_1 = \frac{\kappa_1^2}{s}$$
 (2-10)

For convenience of nomenclature only, the reaction velocity in layer 2 may be defined as:

$$\kappa_2 = K_2 H_2 \tag{2-11}$$

It has units of [L/T]. However, it is not equivalent to the aerobic layer reaction velocities which include diffusion coefficient as well as a reaction rate constant.

With these definitions the layer 1 and 2 equations become:

$$H_{1} \frac{dC_{T_{1}}}{dt} = s \left( f_{d1} C_{T_{1}} - C_{d0} \right) + w_{12} \left( f_{p2} C_{T_{2}} - f_{p1} C_{T_{1}} \right)$$

$$+ K_{L_{12}} \left( f_{d2} C_{T_{2}} - f_{d1} C_{T_{1}} \right) - \frac{\kappa_{1}^{2}}{s} C_{T_{1}} + J_{T_{1}}$$

$$(2-12)$$



$$H_{2} \frac{dC_{T2}}{dt} = w_{12} (f_{d2}C_{T2} - f_{p1}C_{T1}) - K_{L12} (f_{d2}C_{T2} - f_{d1}C_{T1}) - \kappa_{2}C_{T2} - w_{2}C_{T2} + J_{T2}$$
(2-13)

### 2.3.2 Particulate Phase Mixing

The rate of mixing of sediment particles by macrobenthos (bioturbation) has been quantified by estimating an apparent particle diffusion coefficient. The variation has been found to be proportional to the biomass of the benthos (Matisoft, 1982). In addition, it has been found that the benthic biomass is correlated to the carbon input to the sediment (Maughan, 1986, Robbins et al., 1989). In order to make the model self consistent - that is to use only internally computed variables in the parameterization - it seems reasonable to assume that benthic biomass is proportional to the labile carbon in the sediment, which is calculated by the model as  $G_{POC,1}$ . The temperature dependency of particle mixing has been accounted for by using an Arrhenius formulation.

A series of experiments have examined the relationship between particle mixing due to benthic organisms and the overlying water oxygen concentration. There is a general dependency of mixing rate on DO, with the lower rates occurring at the lower DO concentration. This dependency is modeled using a Michaelis Menton expression. The particle mixing mass transfer coefficient that results is:

$$\mathbf{w}_{12}^{*} = \mathbf{D}_{p} \frac{\mathbf{\theta}_{Dp}^{(T-20)}}{\mathbf{H}_{2}} \frac{\mathbf{G}_{POC,1}}{\mathbf{G}_{POC,R}} \frac{\left[O_{2}(0)\right]}{\mathbf{K}_{M,Dp} + \left[O_{2}(0)\right]}$$
(2-14)

with units [L/T]. The superscript \* is used to denote this formulation from the final expression for  $w_{12}$  that is developed below. The parameter values are:

 $D_p$  = Diffusion coefficient for particle (m<sup>2</sup>/d),

 $\theta_{Dp}$  = Temperature coefficient for  $D_p$ 

 $G_{POC,R}$  = Reference concentration for  $G_{POC,1}$  (mg/m<sup>3</sup>),

 $K_{M,Dp}$  = Particle mixing half saturation constant for oxygen (mg/L).

#### 2.3.3 Benthic Stress

In addition to the reduction in particle mixing velocity due to the instantaneous oxygen concentration, it has been found necessary to include a more lasting effect. In particular, if anoxia occurs the benthic fauna population is reduced or eliminated. This is modeled using a first order differential



equation that accumulates stress, S, when overlying water dissolved oxygen is below the particle mixing half saturation constant for oxygen,  $K_{M,Dp}$ . Thus:

$$\frac{dS}{dt} = -k_s S + \frac{K_{M,Dp}}{K_{M,Dp} + [O_2(O)]}$$
(2-15)

where:

S = Accumulated benthic stress [T],

k<sub>s</sub> = First order decay coefficient for accumulated stress [T<sup>-1</sup>].

The behavior of this formulation can be understood by evaluating the limiting steady state stresses at the two oxygen extremes:

$$[O_2(0)] \rightarrow 0 \quad k_s S \rightarrow 1 \quad (1-k_s S) \rightarrow 0$$

$$[O_2(0)] \rightarrow \infty \quad k_s S \rightarrow 0 \quad (1-k_s S) \rightarrow 1$$

Note that as  $[O_2(0)]$  approaches zero at the onset of anoxia, the term  $(1 - k_s S)$  is the proper variable to quantify the degree of benthic stress. The expression is unitless and requires no additional parameter - for example a half saturation constant for benthic stress. The final formulation for the particle mixing velocity which includes the benthic stress is:

$$\mathbf{w}_{12} = \mathbf{w}_{12}^* \min \left\{ (1 - \mathbf{k}_s \mathbf{S}) \right\} \tag{2-16}$$

where  $\mathbf{w}_{12}^*$  is defined above. The stress is continued at its minimum value through the end of the year, in order to conform to the observation that once the benthos has been suppressed by low oxygen, it does not recover until the next year.

### 2.3.4 Dissolved Phase Mixing

Dissolved phase mixing between layers 1 and 2 is via passive molecular diffusion which is enhanced by the mixing activities of the benthic organisms (bio-irrigation). This is modeled by increasing the diffusion coefficient by a factor of 10 over the molecular diffusion coefficient.

$$K_{L12} = \frac{D_d \theta_{Dd}^{(T-20)}}{H_2}$$
 (2-17)



 $D_d$  = Pore water diffusion coefficient (m<sup>2</sup>/day),

 $\theta_{Dd}$  = Temperature coefficient for  $D_d$ .

### 2.3.5 Solids Burial

The deposition of solids to the sediment causes an increase in the depth of the sediment relative to a fixed datum. If the sediment surface is regarded as the point of reference, then the increase in the depth of sediment is a loss of mass due to burial from the active sediment layer.

 $w_2$  = Sedimentation velocity (m/d)

## 2.3.6 Active Layer Depth

The active layer depth is chosen to represent the depth of organism mixing. Particles buried below this depth can longer be recycled to the aerobic layer. They are permanently buried.

 $H_2$  = Depth of the anaerobic layer (m)



Table 2-1. Sediment Model Coefficients

Description	Notation	Value	Units
Aerobic layer solids concentration	$m_1$	0.2-1.2	kg/L
Anaerobic layer solids concentration	$m_2$	0.2-1.2	kg/L
Particle mixing diffusion coefficient	$D_p$	0.00006	$m^2/d$
Sedimentation velocity	$\mathbf{w}_2$	0.25-0.75	cm/yr
Pore water diffusion coefficient	$\overline{\mathrm{D}}_{\mathrm{d}}^{2}$	0.0005-0.0050	$m^2/d$
Temperature coefficient	$\overset{-}{ heta}_{ ext{Dp}}^{ heta}$	1.08-1.10	/ 🐱
Temperature coefficient	$oldsymbol{ heta}_{ ext{Dd}}$	1.10-1.117	
Water-sediment diffusion coefficient	$\mathrm{D}_{\mathrm{d}0}$	0.001	$m^2/d$
Temperature coefficient	$\overset{-}{ heta}_{ ext{D}_{ ext{d}0}}^{ ext{d}0}$	1.08	/
Reaction velocity for nitrification-saltwater		0.1313	m/d
Reaction velocity for nitrification-freshwater	$oldsymbol{\kappa}_{ m nh4}$	0.1313	m/d m/d
Ammonia partition coefficient		1.0	L/kg
Temperature coefficient	$egin{array}{l} \pi_{ m nh4} \  heta_{ m nh4} \end{array}$	1.123	L/ kg
Nitrification half saturation	$\sigma_{\rm nh4}$	1.123	
constant for ammonia	1,-	728.	ma N /I
	$\mathbf{k}_{\mathrm{mnh4}}$	1.125	mg N/L
Temperature coefficient Nitrification half saturation	$ heta_{ m kmnh4}$	1.123	
	1,	0.37	ma O /I
constant for oxygen Aerobic denitrification velocity-saltwater	k <sub>mnh4o2</sub>	1.25	$mg O_2/L$ $m/d$
Aerobic denitrification velocity-freshwater	$\kappa_{ m 1no3}$	0.20	m/d m/d
Anaerobic layer reaction velocity	$\kappa_{1\text{no}3}$	0.25	m/d m/d
Temperature coefficient	$\kappa_{2\text{no}3}$	1.08	111/ U
Reaction velocity for dissolved sulfide	$\theta_{ m no3}$	1.00	
oxidation in the aerobic layer	16	0.2	m/d
Reaction velocity for particulate sulfide	$\kappa_{ m d1}$	0.2	111/ U
	16	0.4	m/d
oxidation in the aerobic layer Partition coefficient for	$\kappa_{p1}$	0.4	111/ U
	T	100.	I /1, 0
sulfide in the aerobic layer Partition coefficient for	$\pi_{1\mathrm{s}}$	100.	L/kg
sulfide in the anaerobic layer	Т	100.	I /lzo
Temperature coefficient	$oldsymbol{\pi}_{2 ext{s}}$	1.08	L/kg
Sulfide oxidation normalization	$\theta_{ ext{dp1}}$	1.00	
	1-	4.	ma O /I
constant for oxygen First order reaction rate	k <sub>mhso2</sub>	0.5-0.75	mg O <sub>2</sub> /L
Silica saturation concentration	$k_{si}$	40000.	/day
	$c_{sisat}$	40000.	μg Si/L
Incremental partition coefficient	۸ =	10	
for silica in the aerobic layer Partition coefficient for	$\Delta\pi_{1 ext{si}}$	10.	
	<b>—</b>	100	I /l-~
silica in the anaerobic layer	$\pi_{2\mathrm{si}}$	100.	L/kg
Depth of sediment layer	$h_{20}$	0.1	m
Temperature coefficient	$oldsymbol{ heta}_{ ext{si}}$	1.10	



Table 2-1. Sediment Model Coefficients (Continued)

Description	Notation	Value	Units
Particulate biogenic silica half			
saturation constant for dissolution	1,-	5.0E+07	$mg Si/m^3$
Overlying water oxygen concentration	$k_{mpsi}$	J.012 + 07	111g 31/ 111
at which aerobic layer incremental			
partitioning starts to decrease	${ m O}_{ m 2critsi}$	2.0	$mg O_2/L$
Partition coefficient for phosphate in the	2critsi	2.0	mg O <sub>2</sub> / L
anaerobic layer	$\pi_1 \mathrm{PO}_{4n}$	20-1000	L/kg
Enhanced aerobic layer partition coefficient	771	20 1000	12/ 11g
under fully oxic conditions	$\pi_1 \mathrm{PO}_{4m}$	20-300	L/kg
Overlying water oxygen concentration		_, _,	/8
at which aerobic layer incremental			
partitioning starts to decrease	${ m O}_{ m 2crit}$	2	$mg O_2/L$
Particle mixing half saturation	ZCIIt		0 2
constant for oxygen	$k_{mo2Dp}$	4.0	$mg O_2/L$
Temperature which benthic community			<u> </u>
begins to recover after an			
anoxic event	tempbnth	10.0	°C
Rate at which benthic stress is dissipated	$k_{bnthstr}$	0.03	/d
Scale factor for enhancement of			
dissolved phase mixing due			
to benthic activity	$k_{lbnth}$	0.0	
Minimum particle mixing coefficient	$\mathrm{D}_{pmin}$	3.0E-06	m2/d
Reaction velocity for methane	$\kappa_{ m ch4}$	0.2	m/d
oxidation in the aerobic layer			
Temperature coefficient	$ heta_{ m ch4}$	1.08	
Reaction Rate Constant for Diagenesis -G1	$k_{GPOM,1}$	0.035	/day
Reaction Rate Constant for Diagenesis -G2	$k_{GPOM,2}$	0.0018	/day
Reaction Rate Constant for Diagenesis -G3	$k_{GPOM,3}$	0.0-1.0E-6	/day
Temperature Coefficient for Diagenesis - G1	$oldsymbol{ heta}_{ ext{G1}}$	1.10	
Temperature Coefficient for Diagenesis - G2	$oldsymbol{ heta}_{ ext{G2}}$	1.15	
Temperature Coefficient for Diagenesis - G3	$oldsymbol{ heta}_{ ext{G3}}$	1.17	



Table 2-1. Sediment Model Coefficients (Continued)

Distribution of Water Water Column POM							
Source	Fractio	ons To Eac	h Class				
	<b>G</b> 1	G2	G3				
Algal Carbon	0.6	0.2	0.2				
Labile Particulate Organic Carbon	1.0	0.0	0.0				
Refractory Particulate Organic Carbon	0.0	0.5	0.5				
Algal Nitrogen	0.6	0.2	0.2				
Labile Particulate Organic Nitrogen	1.0	0.0	0.0				
Refractory Particulate Organic Nitrogen	0.0	0.6	0.4				
AlgalPhosphorus	0.6	0.2	0.2				
Labile Particulate Organic Phosphorus	1.0	0.0	0.0				
Refractory Particulate Organic Phosphorus	0.0	0.5	0.5				



#### **GROUP P: SEDIMENT MODEL INPUT**

P1. Print Options

80

Comment

FORMAT (A80)

Comment | Comment line (ignored by RCA)

10 20 30 40 ISEDPRNT IPRNTSED TWARPSED IGDSEDOPT FORMAT (2I10,6X,A4,I10)

ISEDPRNT = sediment print control

= 0, do not print sediment input

= 1, print sediment input

IPRNTSED = print interval to save sediment computations (nominal = seconds)

TWARPSED = time-warp or units used for IPRNTSED. Normally IPRNTSED

is input in units of seconds. The user may, however, use different

units.

= SECS or secs

= MINS or mins

= HRS or hrs

= DAYS or days

IGDSEDOPT = global dump averaging option

= 0, no averaging

= 1, perform averaging

#### P2. Sediment Depths

80

Comment

FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 80 HSED(1.1) HSED(NY.1)

<u>HSED(1,1)</u> ... <u>HSED(NX,1)</u>

10 8

HSED(1,NY) ... HSED(NX,NY) FORMAT (8F10.0)

HSED(ISED) = sediment layer depth (cm)



#### P3. Sediment Initial Conditions

```
Comment
FORMAT (A80)

Comment = Comment line (ignored by RCA)

\[ \frac{10}{\text{SCALEIC}} \]

FORMAT (F10.0)

SCALEIC = scale factor for each sediment variable initial conditions

\[ \frac{10}{\text{SCARAY}(1,1)} \frac{20}{\text{SCARAY}(2,1)} \frac{80}{\text{SCARAY}(1,NY)} \]

\[ \frac{10}{\text{SCARAY}(1,NY)} \frac{80}{\text{SCARAY}(1,NY)} \]

FORMAT (8E10.0)
```

SCARAY(IX,IY) = sediment initial condition for segment (IX,IY)

The comment line SCALEIC and SCARAY are repeated for each of the following variables used in the sediment nutrient flux model. The order of the initial conditions required for the sediment nutrient flux model is as follows:

```
CTEMP (IX,IY)
                        = Initial sediment temperature (°C)
CPOP (IX,IY, 1)
                        = G<sub>1</sub> Particulate Organic Phosphorus, POP ,(mg/m<sup>3</sup>)
CPON (IX,IY, 1)
                        = G<sub>1</sub> Particulate Organic Nitrogen, PON, (mg/m<sup>3</sup>)
                        = G<sub>1</sub> Particulate Organic Carbon, POP, (mg/m<sup>3</sup>)
CPOC (IX,IY, 1)
CPOP (IX,IY, 2)
                        = G_2 POP (mg/m^3)
                        = G_3 PON, (mg/m^3)
CPON (IX,IY, 2)
CPOC (IX,IY, 2)
                        = G_2 POC, (mg/m^3)
CPOP (IX,IY, 3)
                        = G_3 POP, (mg/m^3)
                        = G_3 PON, (mg/m^3)
CPON (IX,IY, 3)
                        = G_3 POC, (mg/m^3)
CPOC (IX,IY, 3)
                        = Layer 2 orthophosphate, PO<sub>4</sub>, (mg/m<sup>3</sup>)
PO4T2 (IX,IY)
NH4T2 (IX,IY)
                        = Layer 2 ammonia, NH_4, (mg/m^3)
NO3T2 (IX,IY)
                        = Layer 3 nitrate, NO_3, (mg/m^3)
H2ST2 (IX,IY)
                        = Layer 2 hydrogen sulfide (in oxygen equivalents), H<sub>2</sub>S, (mg
                            O_2/m^3
                        = Layer 2 silica, (mg/m^3)
SIT2 (IX,IY)
BNTHSTRS (IX,IY)
                        = Benthic stress
PO4T1 (IX,IY)
                        = Layer 1 orthophosphate, PO_4, (mg/m^3)
NH4T1 (IX,IY)
                        = Layer 1 ammonia, NH_4, (mg/m^3)
```



NO3T1 (IX,IY) = Layer 1 nitrate NO<sub>3</sub>, (mg/m³) SIT1 (IX,IY) = Layer 1 silica, (mg/m³) H2ST1 (IX,IY) = Layer 1 hydrogen sulfide (in oxygen equivalents), H<sub>2</sub>S, (mg  $O_2/m³$ ) CH4T1 (IX,IY) = Layer 1 total methane (in oxygen equivalents), CH<sub>4</sub>, (mgO<sub>2</sub>/m³) CH4T2(IX,IY) = Layer 2 Total Methane (in oxygen equivalents), CH<sub>4</sub>, (mgO<sub>2</sub>/m³) SO4T2 (IX,IY) = Layer 2 total sulfate (in oxygen equivalents), SO<sub>4</sub>, (mgO<sub>2</sub>/m³)

### P4. <u>Temperature Diffusion Coefficient, G Component Fractions and Diagenesis</u> Rates

Comment FORMAT (A80)

Comment | Comment line (ignored by RCA)

DIFFT FORMAT (F10.0)

DIFFT = Water column-sediment layer temperature diffusion coefficient (cm²/sec)

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

SALTSW FORMAT(F10.0)

SALTSW = salinity concentration for determining whether saltwater or freshwater nitrification and denitrification rates are applied.

(If salinity is greater than SALTSW then saltwater values are

applied.

Comment FORMAT (A80)



		nelease 3.0
Comment	=	Comment line (ignored by RCA)
10	20	30
FRPPH1(1) FRP	PH1(2)	FRPPH1(3)
FORMAT (3F10.0)	1	
80	_	
Comment		
FORMAT (A80)		
Comment	=	Comment line (ignored by RCA)
331111111111111111111111111111111111111		33
10 FRPPH2(1) FRP	20 PH2(2) I	30 FRPPH2(3)
FORMAT (3F10.0)	ΓΠΖ(Ζ) Ι	FNFFN2(3)
1 01111111 (01 1010)	'	
80		
	_	
Comment	_	
FORMAT (A80)		
Comment	=	Comment line (ignored by RCA)
10	20	30
		<u>50</u> FRPPH3(3)
FORMAT(3F10.0)	` '	
FRPPHI(I)	=	fractions of algal phosphorus going to G <sub>1</sub> , G <sub>2</sub> , G <sub>3</sub>
		sediment organic phosphorus for algal group I.
80		
Comment	_	
_	_	
FORMAT (A80)		
Comment	_	Comment line (ion and by PCA)
Comment	=	Comment line (ignored by RCA)
10	20	30
FRPOP(1) FRPO	<u>20</u> DP(2) FR	30 POP(3)
FORMAT(3F10.0)		
•		
FRPOP(I)	=	fraction of non-algal/detrital POP going to G <sub>1</sub> , G <sub>2</sub> , G <sub>3</sub>
		sediment organic phosphorus



		11010400 010
80		
Comment		
FORMAT (A80)		
7 07 11717 (7 100)		
Comment	=	Comment line (ignored by RCA)
10	20	30
FRNPH1(1) FRNP		
FORMAT (3F10.0)		
80		
Comment		
FORMAT (A80)		
Comment	=	Comment line (ignored by DCA)
Comment	_	Comment line (ignored by RCA)
10	20	30
FRNPH2(1) FRNP		RNPH2(3)
FORMAT (3F10.0)		
80		
Comment		
FORMAT (A80)		
( ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		
Comment	=	Comment line (ignored by RCA)
10 FRNPH3(1) FRNP	20	30 (DND112(0)
FORMAT(3F10.0)	H3(2) F	RNPH3(3)
1 01 (10.0)		
FRNPHI(I)	=	fraction of algal nitrogen going to G <sub>1</sub> , G <sub>2</sub> , and G
114 (111(1)		sediment organic nitrogen for algal group I
		seament organic introgen for algai group i
00		
80		
Comment		
FORMAT (A80)		
Comment	=	Comment line (ignored by RCA)
4.5		
10 FRPON(1) FRPO	20 N(2) FI	<u>30</u> RPON(3)
FORMAT(3F10.0)	11( <i>L)</i> [[	
. 5 (6. 16.6)		
FRPON(I)	=	fraction of non-algal/detrital PON going to G <sub>1</sub> , G <sub>2</sub> , and
(-)		$G_3$ sediment organic nitrogen
		of occument organic introgen



80 Comment		
FORMAT (A80)		
Comment	=	Comment line (ignored by RCA)
10 FRCPH1(1) FRCF FORMAT (3F10.0)	20 PH1(2) F	30 FRCPH1(3)
Comment FORMAT (A80)		
Comment	=	Comment line (ignored by RCA)
10 FRCPH2(1) FRCF FORMAT (3F10.0)	20 PH2(2) F	30 FRCPH2(3)
Comment FORMAT (A80)		
Comment	=	Comment line (ignored by RCA)
10 FRCPH3(1) FRCF FORMAT(3F10.0)	20 PH3(2) F	30 FRCPH3(3)
FRCPHI(I)	=	fraction of algal carbon going to $G_1$ , $G_2$ , and $G_3$ sediment organic carbon from algal group $I$
Comment FORMAT (A80)		
Comment	=	Comment line (ignored by RCA)
10 FRPOC(1) FRPO FORMAT(3F10.0)	20 DC(2) F	30 RPOC(3)
FRPOC(I)	=	fraction of non-algal/detrital POC going to $G_1$ , $G_2$ , and $G_3$ sediment organic carbon



Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 20 30 40 50 60 <u>KPDIAG(1) DPTHTA(1) KPDIAG(2) DPTHTA(2) KPDIAG(3) DPTHTA(3)</u> <u>FORMAT(6F10.0)</u>

KPDIAG(I) = diagenesis reaction rates for POP  $G_1$ ,  $G_2$  and  $G_3$ , respectively,

DPTHTA(I) = temperature coefficients for POP  $G_1$ ,  $G_2$  and  $G_3$ , respectively

10 20 30 40 50 60 KNDIAG(1) DNTHTA(1) KNDIAG(2) DNTHTA(2) KNDIAG(3) DNTHTA(3) FORMAT(6F10.0)

KNDIAG(I) = diagenesis reaction rates for  $PONG_1$ ,  $G_2$  and  $G_3$ , respectively,

(1/day)

DNTHTA(I) = temperature coefficients for PON  $G_1$ ,  $G_2$  and  $G_3$ , respectively

10 20 30 40 50 60 KCDIAG(1) DCTHTA(1) KCDIAG(2) DCTHTA(2) KCDIAG(3) DCTHTA(3) FORMAT(6F10.0)

KCDIAG(I) = diagenesis reaction rates for POC  $G_1$ ,  $G_2$  and  $G_3$ , respectively,

(1/day)

DCTHTA(I) = temperature coefficients for POC  $G_1$ ,  $G_2$  and  $G_3$ , respectively

10 20 KSI THTASI FORMAT(2F10.0)

KSI = Diagenesis reaction rate for Si, (1/day)

THTASI = Temperature coefficient for Si

P5. Sedimentation and Particle Mixing Rates

Comment FORMAT (A80)

Comment ine (ignored by RCA)



10 20 80 VECTOR(1,1) VECTOR(2,1) ... VECTOR(NX,1) .

:

10 80 <u>VECTOR(1,NY)</u> ... <u>VECTOR(NX,NY)</u> FORMAT(8F10.0)

Comment and VECTOR(IX,IY) are repeated for the following variables:

 $\begin{array}{lll} VSED(IX,IY) & = & sedimentation velocity, (cm/yr) \\ VPMIX(IX,IY) & = & solid-phase mixing rate, (m^2/day) - D_p \\ VDMIX(IX,IY) & = & dissolved-phase mixing rate, (m^2/day) - D_d \end{array}$ 

P6. Sediment Model Constants

Comment FORMAT (A80)

Comment line (ignored by RCA)

<u>10</u> <u>20</u> <u>30</u> <u>M1M2OPT PIESIOPT PIEPO4OPT</u> FORMAT(3F10.0)

M1M2OPT = M1,M2 input option

= 0, M1 and M2 are spatially constant

= 1, M1 and M2 are spatially variable

PIESIOPT = PIESI input option

= 0, Si partition coefficients are spatially constant
 = 1, Si partition coefficients are spatially variable

PIEPO4OPT = PIEPO4 input option

= 0, PO<sub>4</sub> partition coefficients are spatially constant

= 1, PO<sub>4</sub> partition coefficients are spatially variable

If MIM20PT = 0 (spatially constant M1 and M2)

Comment FORMAT (A80)

Comment = Comment line (ignored by RCA)

10 20 30 40 M1 M2 THTADp THTADd FORMAT(4F10.0)



M1 = aerobic layer solids concentration, (kg/l)
M2 = anaerobic layer solids concentration, (kg/l)

THTADp = temperature coefficient for  $D_p$ THTADd = temperature coefficient for  $D_d$ 

If MIM20PT = 1 (spatially variable M1 and M2)

Comment FORMAT (A80)

Comment ine (ignored by RCA)

SCALE FORMAT (F10.0)

SCALE = scale factor

 $\begin{array}{cccc} 10 & 20 & 80 \\ \hline M1(1,1) & M1(2,1) & \dots & M1(NX,1) \\ & & & & \\ \end{array}$ 

.

M1(1,NY) M1(2,NY) . . . M1(NX,NY)

FORMAT(8F10.0)

M1(IX,IY) = aerobic layer solids concentration for sediment segment IX,IY (kg/L)

10 SCALE FORMAT (F10.0)

SCALE = scale factor

. <u>M2(1,NY)</u> <u>M2(2,NY)</u> . . . <u>M2(NX,NY)</u> FORMAT(8F10.0)

M2(IX,IY) = an aerobic layer solids concentration for sediment segment IX,IY (kg/L)



Comment FORMAT (A80)

Comment | = Comment line (ignored by RCA)

10 20
THTADp THTADd

FORMAT (2F10.0)

THTADp = temperature coefficient for  $D_p$ THTADd = temperature coefficient for  $D_d$ 

Comment FORMAT (A80)

Comment | = Comment line (ignored by RCA)

<u>10 20</u> <u>Dd0 THTADd0</u> FORMAT(2F10.0)

Dd0 = minimum pore water diffusion coefficient ( $m^2/day$ )

THTADd0 = temperature coefficient for Dd0

Comment FORMAT (A80)

Comment | Comment line (ignored by RCA)

 10
 20
 30
 40
 50
 60

 KAPPNH4S
 PIENH4
 THTANH4S
 KMNH4
 THTAKMNH4
 KMNH4O2

FORMAT(6F10.0)

KAPPNH4S = nitrification velocity in saltwater, (m/d)
PIENH4 = partition coefficient for nitrogen, (L/kg)

THTANH4S = nitrification temperature coefficient in saltwater KMN4 = ammonia half saturation constant, (mg N/L)

THTAKMN4 = temperature coefficient

KMNH402 = oxygen half saturation constant, (mg  $O_2/L$ )



80 Comment FORMAT (A80)

Comment Comment line (ignored by RCA)

KAPPNH4F THTANH4F FORMAT(2F10.0)

KAPPNH4F nitrification velocity in freshwater, (m/d)

THTANH4F nitrification temperature coefficient in freshwater

80 Comment FORMAT (A80)

Comment Comment line (ignored by RCA)

KAPP1NO3S FORMAT(3F10.0)

KAPP1NO3S = aerobic denitrification velocity in seawater, (m/d) K2NO3S anaerobic layer denitrification rate for seawater, (1/d)

THTANO3S diagenesis temperature coefficient in seawater

80 Comment FORMAT (A80)

Comment Comment line (ignored by RCA)

20 10 30 KAPP1NO3F K2NO3F THTANO3F

FORMAT(3F10.0)

KAPP1NO3F = aerobic denitrification velocity in freshwater, (m/d) K2NO3F anaerobic layer denitrification rate for freshwater, (1/d)

THTANO3F = diagenesis temperature coefficient in freshwater

80 Comment FORMAT (A80)



Comment = Comment line (ignored by RCA)

10	20	30	40	50	60
KAPPD1	KAPPP1	PIE1S	PIE2S	THTAPD1	KMHSO2
FORMAT	(6F10.0)				

KAPPD1 = reaction velocity for dissolved sulfide oxidation in the aerobic

layer, (m/day)

KAPPP1 = reaction velocity for particulate sulfide oxidation in the aerobic

layer, (m/day)

PIE1S = partition coefficient for sulfide in the aerobic layer, (L/kg) PIE2S = partition coefficient for sulfide in the aerobic layer, (L/kg)

THTAPD1 = temperature coefficient for sulfide oxidation

KMHSO2 = sulfide oxidation normalization constant for oxygen,

 $(mgO_2/L)$ 

If PIESIOPT =0 (PIE1SI and PIE2SI are spatially constant)

Comment = Comment line (ignored by RCA)

10	20	30	40	50	60	70	80
CSISAT	PIE1SI	PIE2SI	KSI	THTASI	KMPSI	OCRITSI	JSIDETR
FORMAT	(8F10.0)						

CSISAT = silica saturation concentration, (mg Si/L)

PIEISI = partition coefficient for silica in aerobic layers, (L/kg) PIE2SI = partition coefficient for silica in anaerobic layer, (L/kg)

KSI = first order reaction rate, (1/day)

THTASI = temperature coefficient

KMPSI = half saturation constant, (mg Si/g)

O2CRITSI = overlying water oxygen concentration at which aerobic layer

incremental, partitioning starts to decrease (mg O<sub>2</sub>/L)

ISIDETR = flux of detrital silica, (mg Si/m<sup>2</sup> - d)

If PIESIOPT =1 (PIE1SI and PIE2SI are spatially variable)

Comment FORMAT (A80)



Comment Comment line (ignored by RCA) 10 SCALE FORMAT (F10.0) **SCALE** scale factor PIE1SI(1,1) PIE1SI(2,1) PIE1SI(NX,1) PIE1SI(NX,NY) PIE1SI(1,NY) FORMAT (8F10.0) 80 Comment FORMAT (A80) Comment = Comment line (ignored by RCA) 10 SCALE FORMAT (F10.0) **SCALE** scale factor 10 PIE2SI(2,1) PIE2SI(1,1) 10 80 PIE2SI(NX,NY) PIE2SI(1,NY) FORMAT (8F10.0) PIE1SI(IX,IY) aerobic layer Si partition coefficient (L/kg) PIE2SI(IX,IY) anaerobic layer Si partition coefficient (L/kg) 80 Comment FORMAT (A80) Comment Comment line (ignored by RCA)



10 CSISAT	20 KSI	30 THTASI	40 KMPSI	50 60 O2CRITSI JSIDETR
FORMAT (				
CSISAT			=	silica saturation concentration, (mg Si/L)
KSI			=	first order reaction rate, (1/day)
THTASI			=	temperature coefficient
KMPSI				= half saturation constant, (mg Si/g)
O2CRITS	SI		=	overlying water oxygen concentration at which
				aerobic layer incremental, partitioning starts to
				decrease (mg $O_2/L$ )
JSIDETR	_		=	flux of detrital silica, (mg Si/m² - d)

If PIEPO4OPT =0 (PIE1PO4M and PIE1PO4N are spatially constant)

Comment FORMAT (A80)

Comment | = Comment line (ignored by RCA)

PIE1PO4M PIE1PO4N FORMAT(4F10.0)	O2CI	RIT KMO2DP
- ( )		
PIE1PO4M	=	incremental partition coefficient for phosphate in
		aerobic layer, (L/kg)
PIE1PO4N	=	partition coefficient for phosphate in the anaerobic
		layer, (L/kg)
O2CRIT	=	overlying water oxygen concentration at which
		aerobic layer incremental partitioning starts to
		decrease, (mg $O_2/L$ )
KMO2DP	=	half saturation constant, (mg Si/g)

If PIEPO4OPT = 1 (PIE1PO4 and PIE2PO4 are spatially variable)

Comment FORMAT (A80)

Comment line (ignored by RCA)

10 SCALE FORMAT (F10.0)



**SCALE** scale factor PIE1PO4(2,1) PIE1PO4(1,NY) PIE1PO4(NX,NY) FORMAT (8F10.0) 80 Comment FORMAT (A80) Comment Comment line (ignored by RCA) 10 SCALE FORMAT (F10.0) **SCALE** scale factor PIE2PO4(2,1) PIE2PO4(NX,1) PIE2PO4(1,NY) PIE2PO4(NX FORMAT (8F10.0) PIE1PO4(IX,IY) aerobic layer PO4 partition coefficient (L/kg) = PIE2PO4(IX,IY) anaerobic layer PO4 partition coefficient (L/kg) 80 Comment FORMAT (A80) Comment line (ignored by RCA) Comment 02CRIT KMO2DP

overlying water oxygen concentration at which aerobic layer

half saturation constant for particle mixing (mgO<sub>2</sub>/L)

incremental partitioning starts to decrease (mg O<sub>2</sub>/L)



O2CRIT =

KMO2Dp

Comment FORMAT (A80)

Comment | Comment line (ignored by RCA)

10	20	30	40
TEMPBNTH	KBNTHSTR	KLBNTH	DPMIN
FORMAT(4F10	0.0)		

TEMPBNTH = benthic temperature switch (°C)

KBNTHSTR = benthic stress decay rate constant (1/day) KLBNTH = benthic stress enhancement constant

DPMIN = minimum value for physical benthic mixing,  $(m^2/day)$ 

Comment FORMAT (A80)

Comment | Comment line (ignored by RCA)

10	20	30	40	50
KAPPCH4	THTACH4	KMCH402	KMSO4	SO4OMG
FORMAT(5F	10.0)			

KAPPCH4 reaction velocity for methane production (??/day) =temperature coefficient for methane production THTACH4 = half saturation coefficient for methane production KMCH4O2 = (mg O2/L)KMS04 half saturation coefficient for sulfate (mg/L) = SO4OMG =overlying water sulfate concentration (mg s/L)

Table 2-2 presents a sample input deck for the sediment model coefficient set.



```
TABLE 2-2. SAMPLE INPUT DECK FOR THE SEDIMENT MODEL COEFFICIENT SET
C ISEDPRNT IPRNTSED TWARPSED IGDSEDOPT
              864000
                        SECS
C Sediment depths (cm) 0.00
       0.
                           0.0
                                     0.0
               10.00
       0.
                          10.0
       0.
               10.00
                         10.0
       Ο.
                0.00
                          0.0
                                     0.0
C scale factor / temperature initial conditions (Deg C)
 0.100E+01
                 0.0
                           0.0
                                     0.0
      0.0
              3.2
3.2
                          3.2
       0.0
                           3.2
                                     0.0
       0.0
                 0.0
                           0.0
                                     0.0
C scale factor / G1 POP initial conditions (mg P/m**3)
 0.100E+01
               0.0
                           0.0
                                     0.0
      0.0
       0.0
               1320.
                         1320.
                                     0.0
                       1320.
       0.0
              1320.
                                     0.0
                0.0
                          0.0
      0.0
                                     0.0
C scale factor / G1 PON initial conditions (mg N/m**3)
 0.100E+01
              0.0
      0.0
                           0.0
                                     0.0
       0.0
             12400.
                                     0.0
       0.0
             12400.
                       12400.
                                     0.0
               0.0
                          0.0
       0.0
                                     0.0
C scale factor / G1 POC initial conditions (mg C/m**3)
 0.100E+01
              0.0
      0.0
                          0.0
                                     0.0
                       61400.
       0.0
              61400.
       0.0
             61400.
                       61400.
                                     0.0
0.0 0.0 0.0 0.0 0.0 C scale factor / G2 POP initial conditions (mg P/m**3)
 0.100E+01
               0.0
      0.0
                          0.0
                                     0.0
               8680.
       0.0
              8680.
                        8680.
                                     0.0
                0.0
                          0.0
       0.0
                                     0.0
C scale factor / G2 PON initial conditions (mg N/m**3)
 0.100E+01
      0.0
               0.0
                           0.0
              92700.
       0.0
                       92700.
                                     0.0
                      92700.
       0.0
              92700.
                                     0.0
                 0.0
                          0.0
       0.0
C scale factor / G2 POC initial conditions (mg C/m^**3)
 0.100E+01
      0.0
            410000. 410000.
       0.0
                                     0.0
       0.0
            410000.
                      410000.
                                     0.0
       0.0
                 0.0
                           0.0
C scale factor / G3 POP initial conditions (mg P/m**3)
 0.100E+01
             0.0
      0.0
                      58100.
58100.
       0.0
             58100.
             58100.
0.0
       0.0
                                     0.0
                          0.0
C scale factor / G3 PON initial conditions (mg N/m**3)
0.100E+01
      0.0
            480000.
                     480000.
                                     0.0
           480000.
       0.0
                      480000.
                                     0.0
C scale factor / G3 POC initial conditions (mg C/m^**3)
 0.100E+01
           0.0
       0.0
      0.0 4210000. 4210000.
                                     0.0
       0.0 4210000.
                     4210000.
                                     0.0
                 0.0
                          0.0
C scale factor / Biogenic Si initial conditions (mg Si/m**3) 0.100E+01
      0.0
      0.0 5470000. 5470000.
0.0 5470000. 5470000.
C scale factor / Layer 2 Total Inorganic PO4 (mg P/m**3) 0.100E+01
      0.0
             11500.
                       11500.
      0.0
       0.0
             11500.
                       11500.
       0.0
C scale factor / Layer 2 Total NH4 (mg N/m**3) 0.100E+01
       0.0
              8770.
                        8770.
      0.0
```



```
TABLE 2-2. SAMPLE INPUT DECK FOR THE SEDIMENT MODEL COEFFICIENT SET (Cont.).
          8770. 8770.
0.0 0.0
     0.0
      0.0
                                   0.0
  scale factor / Layer 2 Nitrate (mg N/m**3)
 0.100E+01
      0.0
               250.
                         250.
              250.
      0.0
                       250.
                                    0.0
      0.0
               0.0
                         0.0
                                    0.0
  scale factor / Layer 2 Total Sulfide (as O2 equivalents) (mg O2/m**3)
 0.100E+01
      0.0
                0.0
                          0.0
                                    0.0
      0.0
              1180.
                        1180.
                                    0.0
             1180.
                      1180.
                         0.0
      0.0
               0.0
                                    0.0
C scale factor / Layer 2 Total Inorganic Si (mg Si/m**3)
 0.100E+01
                0.0
                          0.0
                                    0.0
      0.0
      0.0
             22700.
                      22700.
                                    0.0
             22700.
                     22700.
      0.0
               0.0
                          0.0
                                    0.0
C scale factor / Benthic Stress initial conditions
 0.100E+01
      0.
               0.00
                         0.0
                                    0.0
             11.00
                      11.0
      0.
                                    0.0
0. 0.00 0.0 0.0
C scale factor / Layer 1 Total Inorganic PO4 (mg P/m**3)
 0.100E+01
              0.0
     0.0
                          0.0
                                    0.0
                     0.0
16000.
16000.
             16000.
      0.0
                                    0.0
             16000.
      0.0
                         0.0
      0.0
                                    0.0
C scale factor / Layer 1 Total Inorganic NH4 (mg N/m**3)
 0.100E+01
               0.0
                          0.0
                                    0.0
     0.
      0.
               35.0
                          35.
                                    0.0
                          35.
      0.
               35.0
                                    0.0
      0.
                0.0
C scale factor / Layer 1 NO3 (mg N/m**3)
 0.100E+01
     0.
                0.0
                          0.0
                                    0.0
               343.
                         343.
                                    0.0
      0.
               343.
                         343.
                                    0.0
                0.0
                          0.0
      0.
                                    0.0
  scale factor / Layer 1 Total Inorganic Si (mg Si/m**3)
 0.100E+01
               0.0
                          0.0
                                    0.0
     0.
              8000.
      0.
              8000.
                        8000.
                                    0.0
                          0.0
                0.0
      0.
                                    0.0
C scale factor / Layer 1 Sulfide (in oxygen equivalents) (mg O2/m**3)
 0.100E+01
               0.0
                          0.0
                                    0.0
      0.
      0.
               0.02
                        0.02
      0.
               0.02
                         0.02
                                   0.0
                0.0
                          0.0
      0.
                                    0.0
C scale factor / Layer 1 Methane (in oxygen equivalents) (mg O2/m**3)
 0.100E+01
                0.0
                          0.0
                                    0.0
      0.
               0.02
                        0.02
      0.
                                    0.0
                0.0
                          0.0
      0.
                                    0.0
  scale factor / Layer 2 Methane (in oxygen equivalents) (mg O2/m**3)
 0.100E+01
      0.
                0.0
                          0.0
                                    0.0
                          5.0
      0.
      0.
                5.0
                                    0.0
                0.0
                          0.0
      0.
                                    0.0
C scale factor / Layer 2 Sulfate (in oxygen equivalents) (mg 02/m**3)
 0.100E+01
                0.0
      0.
      0.
                0.9
                          0.9
                         0.9
      0.
                0.9
                                    0.0
                0.0
                          0.0
                                    0.0
    Difft
  0.00180
   SALTSW
                                  SALTSW
C FRPPH1-G1 FRPPH1-G2 FRPPH1-G3
                                  fractions to G1, G2, G3 P for Algal Group 1
              0.200
                        0.150
                                  FRPPH1 (G1, G2, G3)
C FRPPH2-G1 FRPPH2-G2 FRPPH2-G3
                                  fractions to G1, G2, G3 P for Algal Group 2
```



```
TABLE 2-2. SAMPLE INPUT DECK FOR THE SEDIMENT MODEL COEFFICIENT SET (Cont.).
     0.650
                 0.200
                            0.150
                                        FRPPH2 (G1,G2,G3)
  FRPPH3-G1 FRPPH3-G2 FRPPH3-G3
                                         fractions to G1, G2, G3 P for Algal Group 3
                                         FRPPH2 (G1,G2,G3)
      0.650
             FRPOP-G2 FRPOP-G3
0.200 0.150
                                       fractions to G1, G2, G3 P for detrital POP FRPOP (G1, G2, G3)
C FRPOP-G1
     0.650
C FRNPH1-G1 FRNPH1-G2 FRNPH1-G3
                                         fractions to G1, G2, G3 N for Algal Group 1
     0.650
                 0.250
                            0.100
                                        FRNPH1 (G1, G2, G3)
C FRNPH2-G1 FRNPH2-G2 FRNPH2-G3
                                        fractions to G1, G2, G3 N for Algal Group 2
                 0.250
                             0.100
                                        FRNPH2 (G1, G2, G3)
      0.650
C FRNPH3-G1 FRNPH3-G2 FRNPH3-G3
                                        fractions to G1, G2, G3 N for Algal Group 3 FRNPH2 (G1,G2,G3)
                 0.250
     0.650
                            0.100
C FRPON-G1 FRPON-G2 FRPON-G3
                                       fractions to G1, G2, G3 N for detrital PON
                                        FRPON (G1,G2,G3)
fractions to G1, G2, G3 C for Algal Group 1
     0.650
                 0.250
                            0.100
C FRCPH1-G1 FRCPH1-G2 FRCPH1-G3
                                        FRCPH1 (G1, G2, G3)
      0.650
C FRCPH2-G1 FRCPH2-G2 FRCPH2-G3
                                        fractions to G1, G2, G3 C for Algal Group 2 FRCPH2 (G1, G2, G3)
     0.650
                 0.200
                            0.150
                                       fractions to G1, G2, G3 C for Algal Group 3 FRCPH2 (G1,G2,G3) fractions to G1, G2, G3 C for detrital POC
C FRCPH3-G1 FRCPH3-G2 FRCPH3-G3
0.650 0.200 0.150
C FRPOC-G1 FRPOC-G2 FRPOC-G3
                                      FRPOC (G1,G2,G3)
THETAG2 KPDIAGG3
1.150 0.0000010
                 0.200
                            0.150
              THETAG1 KPDIAGG2
1.100 0.0018000
C KPDTAGG1
                                                             THETAG3
                                                                          POP Diag Rates
 0.0350000
                                                               1.170
                 HETAG1 KNDIAGG2
1.100 0.0018000
                                      THETAG2 KNDIAGG3
1.150 0.0000010
              THETAG1
                                                             THETAG3
                                                                          PON Diag Rates
C KNDIAGG1
 0.0350000
                                                               1.170
              THETAG1
                                      THETAG2 KCDIAGG3
C KCDIAGG1
                                                             THETAG3
                                                                          POC Diag Rates
                        KCDIAGG2
 0.0350000
                 1.100 0.0018000
                                        1.150 0.0000010
                                                               1.170
                THETA
C KSiDiag
                                                                     Biogenic Diag Rate
    0.500
                 1.100
    Sedimentation or Burial Rates (cm/yr)
C Scale Factor
 0.100E+01
        0.
                 0.00
                              0.0
                                           0.0
                             0.25
        0.
                                           0.0
        0.
                 0.250
                             0.25
                                           0.0
        Λ
                  0.00
                               0.0
                                           0.0
    Particle or solid phase mixing rate (m2/day)
C Scale Factor
 0.100E+01
       0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.120E-03
                                           0.0
        0.0 0.120E-03 0.120E-03
                                           0.0
    0.0 0.0 0.0 0.0 0.0 Dissolved phase mixing rate (m2/day)
                                           0.0
C Scale Factor
 0.100E+01
       0.0 0.100E-02 0.100E-02
0.0 0.100E-02 0.100E-02
                                          0.0
                                          0.0
                    0.0
  M1M2OPT PIESIOPT PIEPO4OPT
                                      (0=spatially constant,1=variable)
                    P1 ...
0 ...
M2 ThetaDp
1500
          0
     0.500
                 0.500
                          1.1500
                                       1.1500
       Ddo
             ThetaDdo
    0.0010
                1.0800
                         ThetaNH4S KMNH4 ThtaKmNH4 KMNH402
1.0800 728.0000 1.1250 0.7400
(freshwater values)
C KappNH4S
                PIENH4 ThetaNH4S
                                                                          (saltwater values)
                1.0000
    0.1313
C KappNH4F ThetaNH4F
    0.2000
                1.0800
                K2NO3S ThetaNO3S
C KappN03S
                                       (saltwater values)
    0.0500
                0.1000
                           1.3000
C KappNO3F
                K2NO3F ThetaNO3F
                                       (freshwater values)
                         1.0800
                0.2500
    0.1000
    Kappd1
0.2000
                Kappp1 0.4000
                            PIE1S
                                        PIE2S ThetaPD1
                         100.0000
                                     100.0000
                                                   1.0800
                                                              4.0000
                                                 ThetaSi
    CSiSat
                PIE1Si
                           PIE2Si
                                          KSi
                                                               KMPSi
                                                                       02CritSi
                                                                                    JsiDetr
             15.000
PIE1PO4N
40000.0000
                            100.00
                                       0.5000
                                                  1.1000
                                                                         2.0000
  PIEPO4M
                           02Crit
                                       KM02Dp
                  20.0
      20.0
                              2.00
                                         4.00
C TempBnth
              KBnthStr
                            KlBnth
   10.0000
               0.0300
                            0.0000
                                       0.0000
                                        KMSO4
   KappCh4
              ThetaCh4
                          KMCH402
                  1.08
                             0.20
       0.20
```



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# APPENDIX B PATHOGEN MODEL

#### PATHOGEN MODEL

Despite significant efforts and expenditures by federal, state, and local government to reduce the sources of pathogenic bacteria, associated with human health risks and diseases, to receiving waters, pathogens continue to be an issue when trying to meet the "swimmable" goals of the Clean Water Act. This is particularly the case for waters that receive combined sewer overflows (CSOs) from the nation's larger and older cities, wherein both sanitary and stormwater are conveyed in the same sewer system. However, modeling of the major waterborne pathogens of concern (including *V. Cholerae, Salmonellae, and Shigella* species) is usually not practiced due to the difficulty in measuring these organisms directly in the receiving waters. Rather surrogate indicator organisms, such as total and fecal coliform are modeled. More recently, through the Coastal Health Act of 2000, the USEPA is requiring that the coastal states implement the enterococci criteria for marine waters originally developed in the 1986 "Ambient Water Quality Criteria for Bacteria - 1986" guidance document. Therefore, the pathogen model developed by HydroQual includes state-variables for total and fecal coliform and enterococcus.

The mathematical framework employed in the pathogen model is the same mass-balance approach detailed in Appendix A - Integrated Eutrophication and Sediment Nutrient Flux Model, only the state-variables and reaction rates differ. The pathogen model includes the following state-variables:

- 1. Salinity (ppt)
- 2. Tracer (mg/L)
- 3. Total Coliform Bacteria (#/100 mL)
- 4. Fecal Coliform Bacteria (#/100 mL)
- 5. Enterococci (#/100 mL)

Note: when inputting loads of coliform bacteria or enterococci, the user should use the following procedure:

bacterial load = wastewater (or CSO) flow \* coliform concentration \* conversion factor

where the coliform concentration is in units of #/100 mL and the conversion factor is:

Units of wastewater flow	Conversion factor
m³/day	0.001
m <sup>3</sup> /sec	86.4
MGD	3.785
cfs	2.446

At the present time, the HydroQual pathogen model only incorporates a first-order decay or die-off rate for coliform bacteria and enterococcus. The model does not account for any post-discharge growth of the organisms in the receiving water. The tracer variable is included in the model framework should the user wish to "tag" or follow the spatial distribution of a particular WWTP(s), CSO(s), or separate sewer overflow (SSOs). The present framework permits the coliform/enterococcus die-off rate to be a function of temperature, sunlight, and, for estuarine/coastal systems, salinity. The following equation represents the die-off rate for total and fecal coliform and entrerococcus:



$$\mathbf{k}_{\text{die-off}} = (\mathbf{k}_{\text{base}} + \mathbf{k}_{\text{sal}}(\mathbf{S})) \cdot \mathbf{\theta}_{\text{sal}}^{(T-20)} + \mathbf{k}_{\text{light}} \cdot \mathbf{f}(\mathbf{I})$$
(1)

where:

composite die-off rate (/day),  $k_{\text{die-off}}$ base die-off rate (/day), k<sub>base</sub> salinity dependent die-off rate (/ppt-day),  $k_{sal}$ S concentration of salinity (ppt), θ temperature correction coefficient for die-off rate, Т temperature (deg C), light-dependent die-off rate (ly-day), = depth- and time-integrated light intensity (ly). f(I)

The function, f(I), may be evaluated as follows:

$$f(I) = \frac{I_0(t)}{K_e H} (1 - \exp(-K_e H))$$
 (2)

where:

 $I_0(t) \hspace{1cm} = \hspace{1cm} \text{solar radiation at water surface (or at surface of model segment if water column is vertically segmented), (ly),} \\ K_e \hspace{1cm} = \hspace{1cm} \text{extinction coefficient (/m),} \\ H \hspace{1cm} = \hspace{1cm} \text{depth of water column (or depth of model segment if the water column is vertically segmented in the model) (m).}$ 

The following presents the structure of the parameters, constants, and time-variable functions input file for running the pathogen model.

#### 2-D Parameters

Number	<u>Name</u>	<u>Descrip</u>	ption
1	KEBS	=	extinction coefficients (used when KEOPT = 1 or 3) $(/m)$ ,
Constants <u>Number</u>	<u>Name</u>	Descrij	<u>ption</u>
1	KCBC	=	base die-off rate for coliform bacteria at 20 deg C (/day),
2	KCBT	=	temperature correction coefficient,
3	KCSAL	=	salinity-dependent coliform die-off rate (/ppt-day),
4	KCLGHT	=	sunlight-dependent coliform die-off rate (/ly-day),
5	SOLAR	=	option to include sunlight-dependent die-off rate, = 0, do not include sunlight effects on die-off rate, = 1, include sunlight effects on die-off rate,
6	KEBC	=	base die-off rate for enterococcus at 20 deg C (/day),
7	KEBT	=	temperature correction coefficient,
8	KESAL	=	salinity-dependent enterococcus die-off rate (/ppt-day),



9 10	KELGHT KEOPT	= =	sunlight-dependent coliform die-off rate (/ly-day), method for inputting extinction coefficients, = 0, K <sub>e</sub> is a constant (i.e., spatially and temporally invariant), = 1, K <sub>e</sub> is spatially variable, but constant in time (uses the 2-D parameter, KEBS) = 2, K <sub>e</sub> is time-variable (uses the time-variable function KETVF), but spatially invariant, = 3, K <sub>e</sub> is spatially variable and can vary in time, using the 2-D parameter, KEBS, and the time-variable function, KETVF,
11	KECONST	=	<ul> <li>4, K<sub>e</sub> is fully variable in time and space, with input coming from a separate input file (kebs.inp),</li> <li>base extinction coefficient (used when KEOPT = 0 or 2) (/m),</li> </ul>
Time-Varial	ble Functions		
<u>Number</u>	<u>Name</u>	Descr	iption
1	ITOTSF	=	total daily solar radiation (used when KEOPT = $2,3$ or $4$ ) (/m),
2	F	=	fraction of daylight (used when KEOPT = 2, 3, or 4),
3	KETVF	=	time-variable scaling factor for extinction coefficients (used when $KEOPT = 2 \text{ or } 3$ ).



# APPENDIX C RESIDENCE TIME/TRACER MODEL

#### RESIDENCE TIME/DYE-TRACER SUBROUTINE

One method for determining whether the transport fields computed by the hydrodynamic model, which are to be used to advect and disperse water quality variables of interest within RCA, are correct is to compare them to observed data. For estuarine systems, these comparisons are usually made using observed water elevations, current meter data, and salinity, temperature, and density data. However, in addition, in special cases tracers, such as Rhodamine dye or SF<sub>6</sub> (sulfur hexafluoride, are used to provide data sets for calibration of hydrodynamic models, particularly when applied to freshwater systems.

In addition, it is often useful to know the residence time of a region or portion of a waterbody. This information can be used to estimate how quickly a contaminant is flushed from that region or portion of the study domain. One way of determining the residence time of the region of interest is to perform model simulations using "conservative tracers or dyes."

Therefore, a TUNER subroutine has been developed that can be used to simulate the transport of a tracer within a study domain and that can be used to estimate the residence time of the tracer within a portion of the model domain or within the entire model domain. The mathematical framework employed in the tracer model is the same mass-balance approach detailed in Appendix A - Integrated Eutrophication and Sediment Nutrient Flux Model, only the state-variables differ. The tracer model has only one state-variable - the tracer or dye (actually the code provided can be quickly expanded to include three tracers or dyes by "un-Commenting" some of the FORTRAN code):

#### 1. Tracer (mg/L)

The residence time or dye model is set up so that, in addition to putting a tracer or dye within the entire model domain, one can initialize only a portion of the model domain with the tracer and then have the model determine (1) the mass of tracer remaining within the initialized portion of the model domain, (2) a user specified portion of the model domain, as well as, (3) the mass of tracer left within the entire model domain. One can then post-process the model outputs to estimate the residence time of the dye using the commonly accepted definition of one e-folding time (one e-folding is defined as exp(-1) or the time at which 0.3679 of the initial mass remains within the region or the study domain).

The following presents the structure of the parameters, constants, and time-variable functions input file for running the pathogen model.

3-D Parameters Number	<u>Name</u>	Descri	<u>ption</u>
1 2	DYE1IC3 DOMAIN1	= =	initial conditions for tracer or dye (mg/L), region of interest for determining residence time
2-D Parameters Number	<u>Name</u>	Descri	<u>ption</u>
1 2	DYE1IC2 DOMAIN1	= =	initial conditions for tracer or dye (mg/L), region of interest for determining residence time



Constants Number	<u>Name</u>	Description
1	DYEDIS1	<ul> <li>dye distribution option,</li> <li>0, assign initial tracer concentrations uniformly in the vertical plane of the model as determined by the 2-D parameter DYE1IC2</li> </ul>
		<ul> <li>= 1, assign initial tracer concentrations on a model segment by model segment basis as determined by the</li> <li>3-D parameter DYE1IC3 (permits one to look at residence time of surface layer versus bottom layer)</li> </ul>
2	TIMEDYE1	= time to release the tracer or dye (days),
3	DECAY1	= decay rate of tracer or dye (1 day)

#### Time-Variable Functions

No time-variable functions are required.



### **APPENDIX D**

## DESCRIPTION OF RCA OUTPUT FILE FORMATS

# FILE DESCRIPTIONS FOR RCAF OUTPUT FILES VERSION 3.0 OF RCA

The water quality modeling program, RCA, creates a number of output files (known as RCAF files) containing various types of model computations that (1) can be visualized by the user via GDP or other post-processing software, (2) can be used to "cycle" model runs, and (3) can provide for mass balance and flux balance analyses of a system. Currently there are four types of files saved by RCA: (1) global dump or map files, (2) detailed dump or history files, (3) "end of simulation" concentration files, and (4) mass balance and flux balance files. The global or map file provide a snapshot of the entire model domain for the key water quality variables, while the detailed or history file provides more "detailed" information about the model simulation for a more limited number of model segments within the model domain. The "end of simulation" concentration files contain the concentrations for all model segments for all systems at the end of the simulation. These files can be used by the user to cycle or "hot-start" a subsequent simulation, if one desires the model to achieve a "new" dynamic equilibrium in response to reductions in pollutant inputs or a management scenario. The mass balance/flux balance files provide information that permits a user to develop a mass balance analysis for a system or to perform a flux balance analysis in a certain portion(s) of the model domain. In order to restrain the physical size of each of the RCAF files, and thus reduce required physical disc-size requirements, all RCAF files are written in binary (rather than ASCII format). The following provides a more detailed description of the content and 'format' of each of the RCAF output files.

#### Global Dump Files - RCAF10 and RCAF11

The RCAF10 file provides information concerning the size of the model, the number of systems, the number of global dumps saved, the variable names, and the times for which the global information was saved. The RCAF11 file contains the concentrations of the key water quality variables within the model domain.

#### RCAF10 (internal RCA file number 10)

Record 1: NX,NY,NZ,NOSYS,NGDMP

where: NX number of computational elements in the x-direction (Integer)
NY number of computational elements in the y-direction (Integer)

NZ number of vertical layers (Integer)

NOSYS number of state-variables in the model (Interger)

NGDMP number of global dumps saved by the kinetic subroutine in RCAF11 (Integer)

Record 2: SYNAME(NGDMP)

where: SYNAME a vector (NGDMP elements long) that contains the names of the water quality

parameters saved in the RCAF11 file (Character\*8)

Record 3: SYSGDP(40)

where: SYSGDP a vector (40 elements long) that contains the system bypass information for

the model run (Integer\*2). Used primarily by HydroQual's in-house post-

processing software.



Record 4: FSM(NX,NY)

where: FSM an array (NX x NY) containing the land-mask information for the model grid

(Real). The following convention is used: water=1, land=0, boundaries=-1 or -2.

Records 5 -> TIME

where: TIME times at which the global dumps were written to the disk. Number of records =

(total length of the simulation time ÷ global dump interval) + 1 (for the initial

conditions).

#### RCAF11 (internal RCA file number 11)

Records 1 -> CARAY

where CARAY arrays (each NX x NY x NZ) containing the concentrations for each model segment in the model domain for each water quality variable of interest (Real). Record 1 contains the CARAY for variable 1, record 2 for variable 2, ..., record NGDMP for variable NGDMP.

Record NGDMP+1 starts with variable 1 again, but for the next time record.

#### Detailed Dump Files - RCAF12 and RCAF13

#### RCAF12 (internal RCA file number 12)

Record 1: NDMPS

where NDMPS number of segments selected for saving detailed dumps (Integer).

Record 2: ((IFDMPS(I,J),J=1,3),I=1,NDMPS)

where IFDMP(I,I) contains the x cell number (j=1), the y cell number (j=2), and the z or sigma-layer

cell number (j=3) for each of the segments saved (Integer).

Record 3: DDGDPBY(40)

where: DDGDPBY a vector (40 elements long) that contains the system bypass information for

the model run (Integer\*2). Used primarily by HydroQual's in-house post-

processing software.

Record 4: DDNAMES(NOSYS,5)

where: DDNAMES a vector (NOSYS x 5 elements long) that contains the names of the water

quality parameters saved in the RCAF13 file (Character\*8). Each model system or state-variables has provision for saving 5 pieces or information (state-variable concentrations, combinations of state-variables, reaction terms, etc.). The specific information saved for each system is determined in the user's kinetic subroutine

TUNER.

Record 5 -> TIME

where: TIME times for which the detailed dumps were saved (Real).



#### RCAF13 (internal RCA file number 13)

Records 1 -> BUFFER(50000)

where: BUFFER an array (50000 elements long) containing the detailed dumps (Real). The

information for each system is packed into the 'buffer' as follows (assume

NOSYS=25):

BUFFER(1-5) = the five pieces of information for the first IFDMP for system 1 BUFFER(6-10) = the five pieces of information for the first IFDMP for system 2

.

BUFFER(121-125) = the five pieces of information for the first IFDMP for system 25 BUFFER(126-130) = the five pieces of information for the second IFDMP for system 1 BUFFER(131-135) = the five pieces of information for the second IFDMP for system 2

.

BUFFER(246-250) = the five pieces of information for the second IFDMP for system 25 BUFFER(251-255) = the five pieces of information for the third IFDMP for system 1 BUFFER(256-260) = the five pieces of information for the third IFDMP for system 2 etc.

Note: not all of the buffer will be used, only NDMPS\*5\*NOSYS elements contain actual model computations (the remaining values should be zero).

#### Sediment Dump File - RCAF14

The RCAF14 file contains information from the sediment flux model (SFM) if used. RCAF14 looks like a global dump or map file, since it contains information generated by the SFM for all active model segments in the model domain (note: only the water segments corresponding to FSM(I,J)=1).

#### RCAF14 (internal RCA file number 14)

Record 1: FSM(NX,NY)

where: FSM an array (NX x NY) containing the land-mask information for the model grid

(Real). The following convention is used: water=1, land=0, boundaries=-1 or -2.

Records 2 ->  $TIME_{,(SED(I),I=1,76)}$ 

where: TIME times at which the SFM info was saved (REAL)

SED a vector (76 elements long) containing information generated by the sediment flux

model (REAL). The SED information is written for each active (FSM=1) segment

using the following DO-loop sequence:

DO ICOL=1,NY
DO IROW=1,NX
WRITE(14) TIME,SED
ENDDO
ENDDO



The following NAMES have been assigned to the SED vector:

SED(1-5): ctemp,pop1r,pop2r,pop3r,popr SED(6-10): pon1r,pon2r,pon3r,ponr,poc1r SED(11-15): poc2r,poc3r,pocr,po4t2r,hst2r SED(16-20): sit2r,psiavr,jpop,jpon,jpoc SED(21-25): o20,csod,sod,s,jdiagp

SED(26-30): jdiagn,jdiagc,jo2nh4,xjco2av,xjc1av

SED(31-35): jpo4,jnh4,jno3,jhs,jsi SED(36-40): jch4aq,jch4g,h1,po40,po41

SED(41-45): po42,po4t2,nh40,nh41,nh42 SED(46-50): nh4t2,no30,no31,no32,no3t2

SED(51-55): hs1,hs2,hst2,si0,si1

SED(56-60): si2,sit2,bnthden,ch41,ch42 SED(61-65): ch4t2,so41,so42,so4t2,flxpopG1

SED(66-70): flxpopG2,flxpopG3,flxponG1,flxponG2,flxponG3 SED(71-75): flxpocG1,flxpocG2,flxpos,flxpos,flxpo4t2s

SED(76): flxsit2s

#### RCA "Hot-Start" Files - RCAFIC and RCAFICSED

The RCAFIC file is used to save the "end of simulation" water column concentrations for use as initial conditions if the user chooses to perform a cycled (or "hot-start") run, while the RCAFICSED file contains similar information but for the sediment nutrient flux model (if used).

#### RCAFIC (internal RCA file number 15)

Record 1: CARAY

where CARAY an array (NX x NY x NZ x NOSYS) containing the concentrations for each model

segment/system in the model domain (NX x NY x NZ) for each water quality variable

(NOSYS) (Real)

#### RCAFICSED (internal RCA file number 16)

Record 1: CTEMP, CPOP, CPON, CPOC, CPOS, PO4T2, NH4T2, NO3T2, H2ST2, SIT2,

BNTHSTRS, PO4T1, NH4T1, NO3T1, SIT1, H2ST1, CH4T1, CH4T2, SO4T2, PO41, NH41, NO31, H2S1, SI1, O2O, SOD, DDO, BFORMAXS, ISWBNTHS

where "array" are arrays (NX x NY x NZ), as listed above, containing the sediment bed

concentrations, benthic stress, SOD, overlying water column, depth of aerobic layer

for each sediment model segment (Real)

#### RCA Flux Balance/Mass Balance Files - RCAFMB and RCAMBSED

Should the user chose to perform flux balance/mass balance computations for an RCA simulation, the requested information will be written to RCAFMB for the water column and RCAMBSED for the sediment nutrient flux model if it is used in the model computations.

#### RCAFMB (internal RCA file number 17)

Records 1 -> TIME, SYSMASS, SYSLOADS, FLXMB, FLYMB

where TIME is the time at which the flux balance/mass balance computations are being written, a vector (NOSYS) containing the total mass for each system in the model(Real).



SYSLOADS an array (4,NOSYS) containing the total mass loading rate (g/day) for each

system in the model. These loading rates are point source, nonpoint source, fall-

line, and atmospheric, respectively.

FLXMB an array (NX x NY) containing the depth-integrated flux terms (mg/day) for each

X-interface in the model

FLYMB an array (NX x NY) containing the depth-integrated flux terms (mg/day) for each

Y-interface in the model

Record 1 contains the mass balance/flux balance terms at the start of the mass balance/flux balance computations, while records 2 and forward contain the same computations written at an interval selected by the user.

#### RCAFMBSED (internal RCA file number 18)

Records 1 -> TIME, TOTORGP, TOTORGN, TOTORGC, TOTBSI, TOTPO4, TOTNH4,

TOTNO3, TOTSI, TOTH2S, TOTCH4, TOTSO4, JPOP, JPON, JPOC, JBSI, JPO4SS, JSISS, BURIALORGP, BURIALORGN, BURIALORGC, BURIALBSI, BURIALPO4, BURIALNH4, BURIALNO3, BURIALSI, BURIALH2S,

BURIALCH4, BURIALSO4, TOTJPO4, TOTJN4, TOTNHO3, TOTHN2, TOTJSI,

TOTJH2S, TOTJCH4AQ, TOTHCH4G, TOTSOD

where TIME is the time at which the flux balance/mass balance computations are being written,

"arrays" arrays (NX x NY) containing the total mass or flux rate, as listed above, for each

relevant system of the sediment flux model (Real).

Record 1 contains the mass balance/flux balance terms at the start of the mass balance/flux balance computations, while records 2 and forward contain the same computations written at an interval selected by the user.

#### **Internal RCA Files**

In addition to the files listed about, RCA utilizes a number of input files and/or temporary files for saving intermediate computations. The following file numbers are reserved by RCA for use as input files:

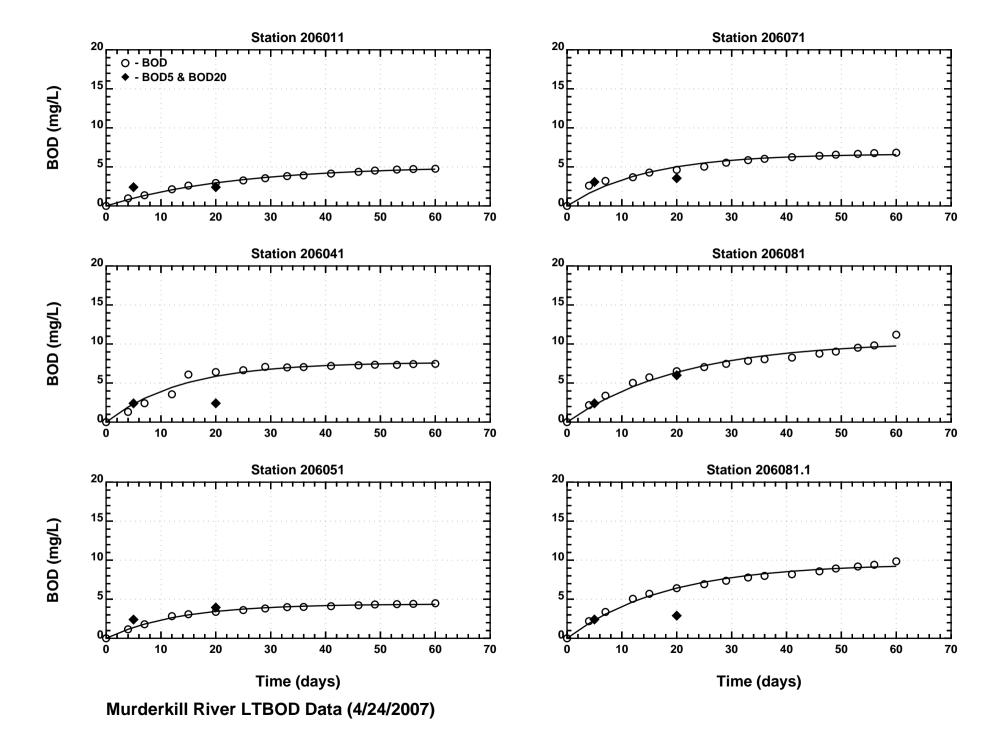
- 30 gcm geom, wet grid, and the hydrodynamic transport file(s) HYDFILNA
- 31 the diffuser file (DIFFILNA) generated by the hydrodynamic model
- 32 the boundary condition file (BCFILNA)
- 33 the point source file (PSFILNA)
- 34 the nonpoint source file (NPSFILNA)
- 35 the fall-line source file (FLFILNA)
- 36 the atmospheric source file (ATMFILNA)
- 37 the parameters, constants, and time-variable functions input file (PCFILNA)
- 38 the initial conditions file (ICFILNA).

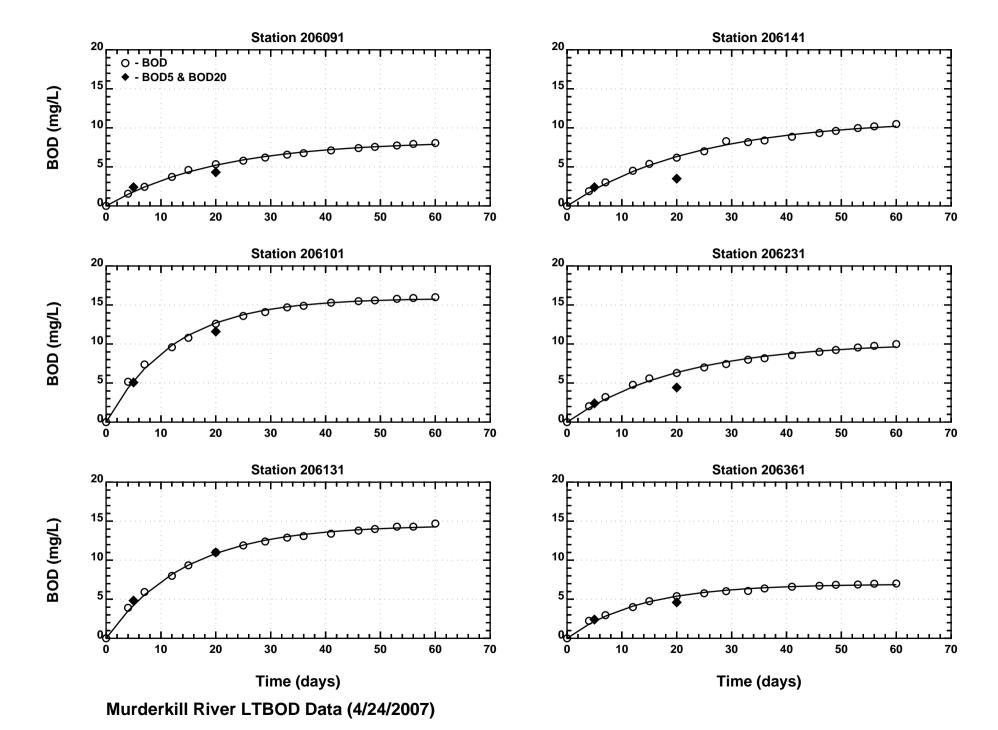
When developing new kinetic subroutines, the model develop should be aware of the file numbers already "assigned" by RCA and should be careful not to assign "new" files to existing file numbers (i.e., 10-18 and 30-38).

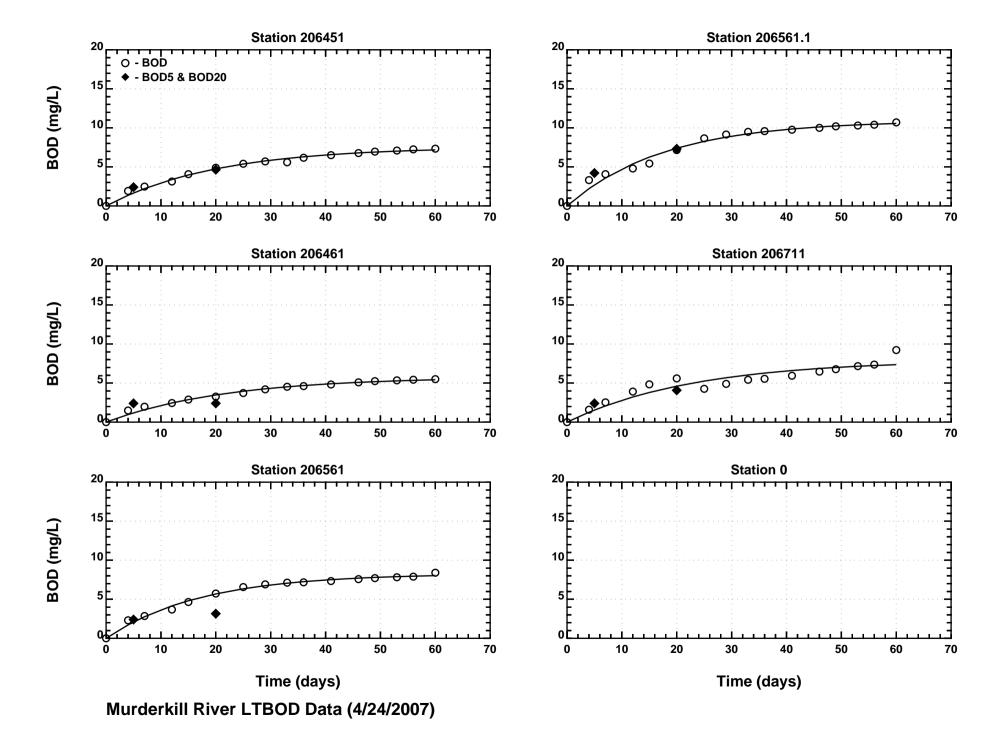


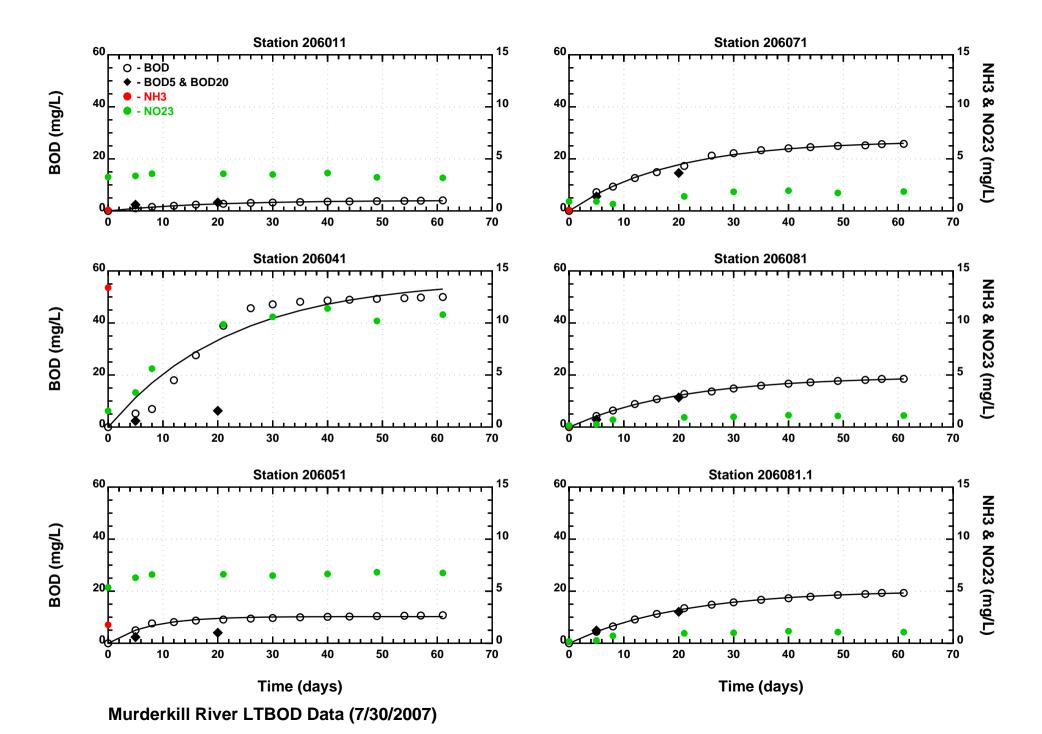
## **APPENDIX 8**

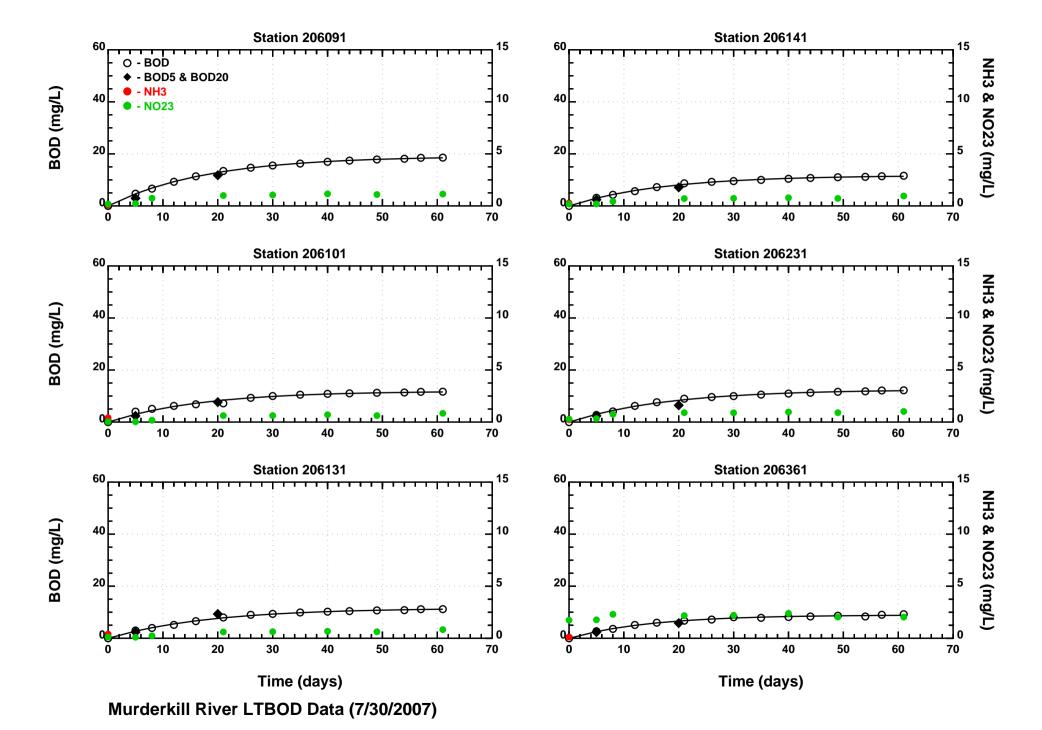
## LTBOD RESULTS FOR RIVER SITES

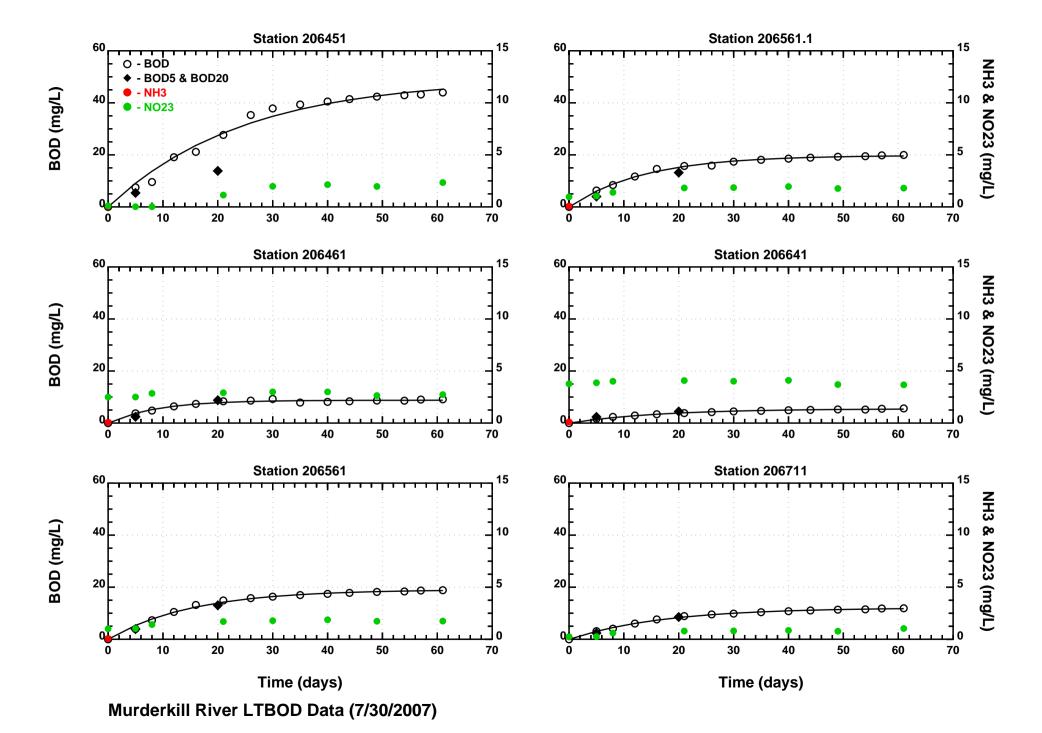


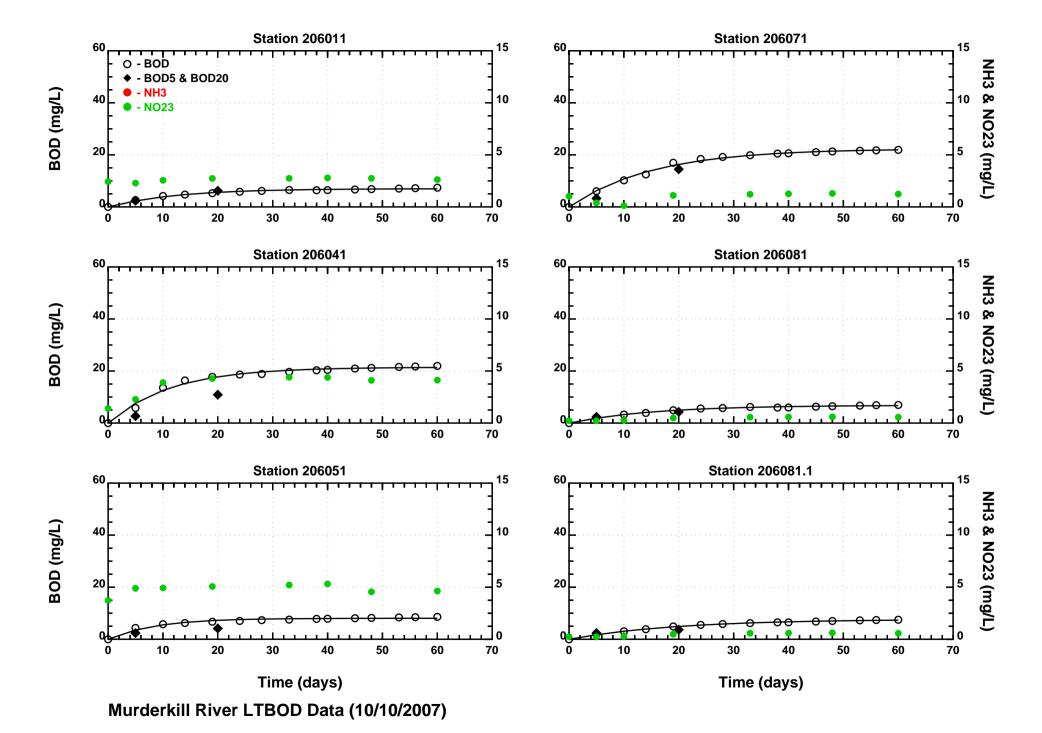


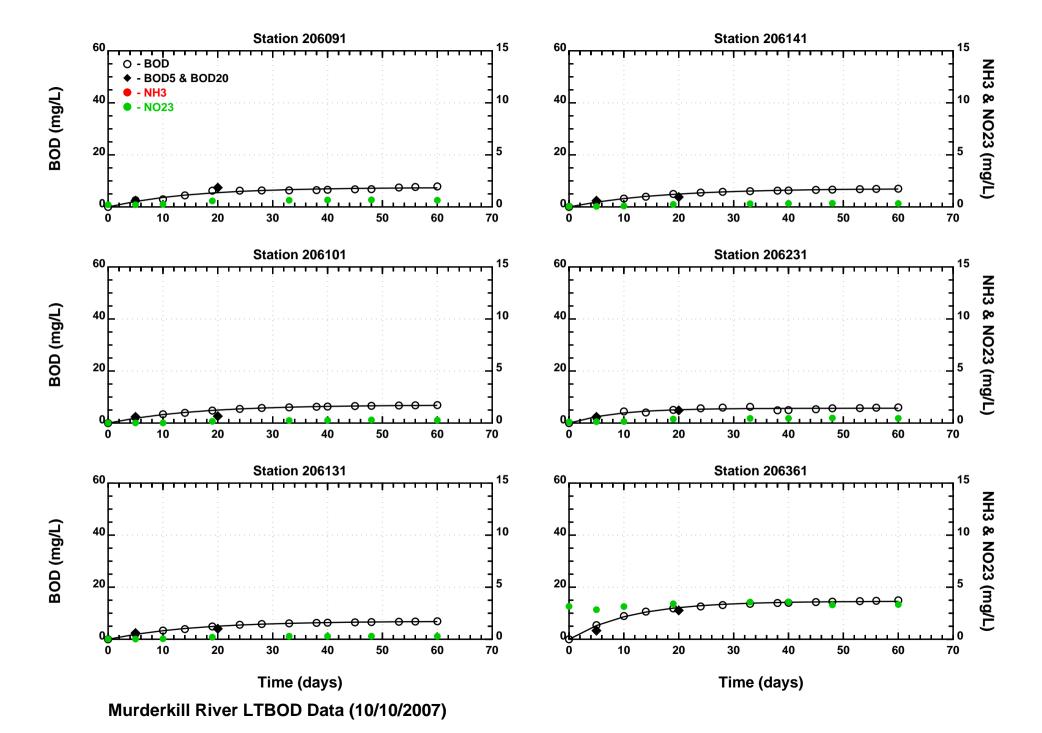


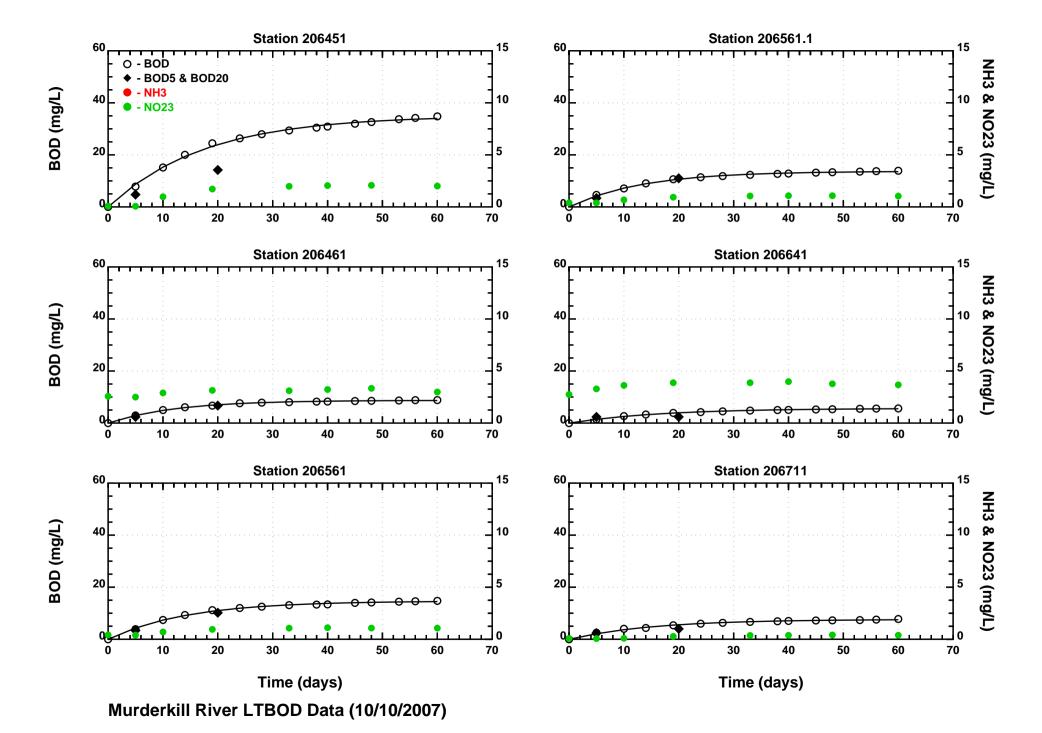


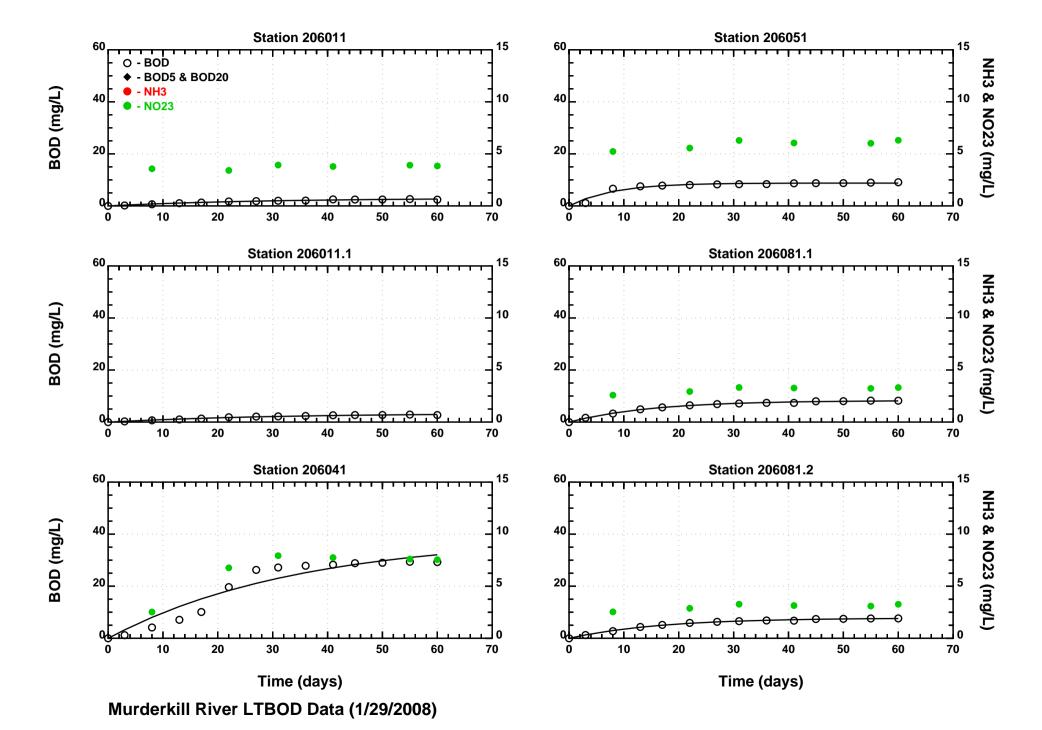


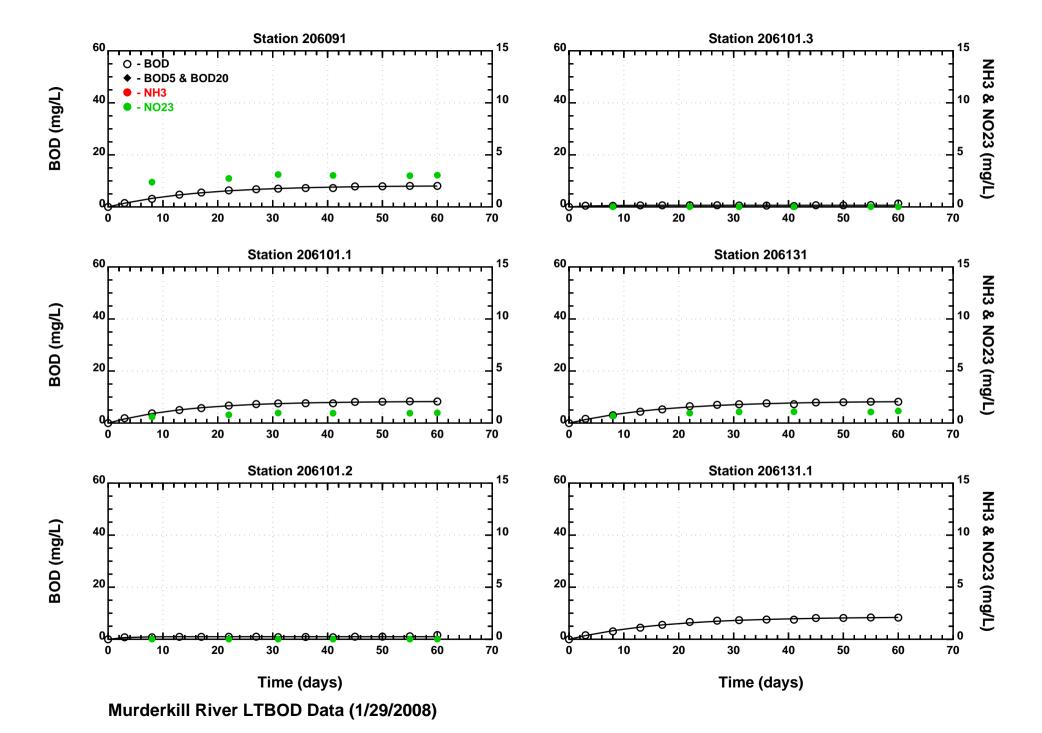


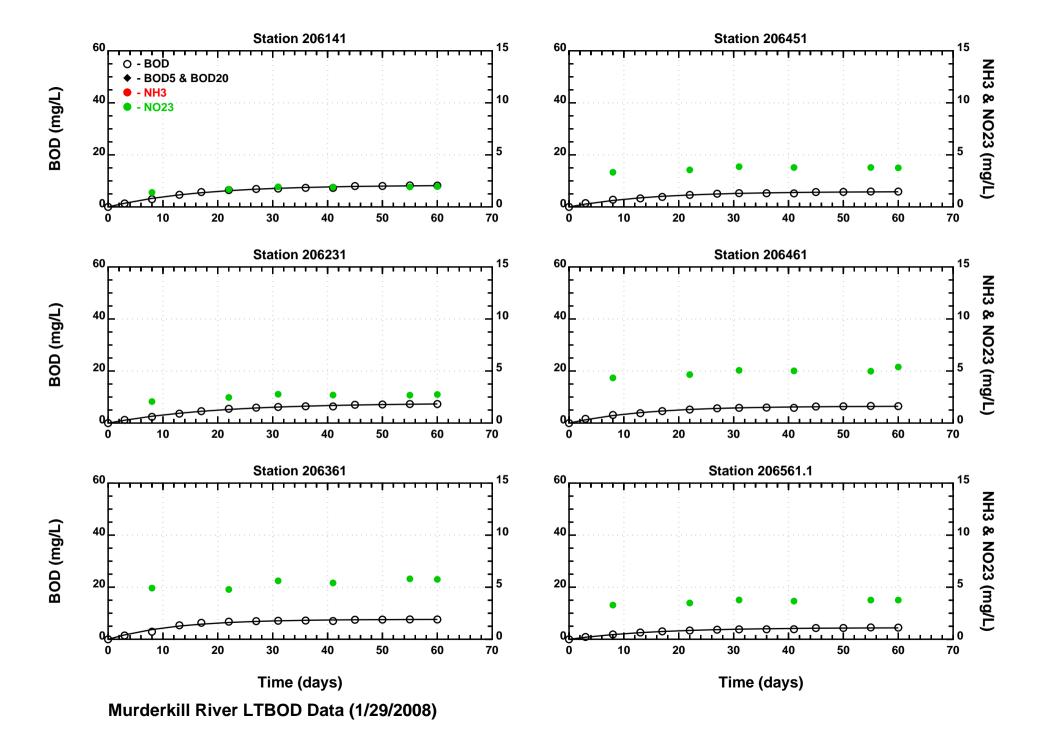


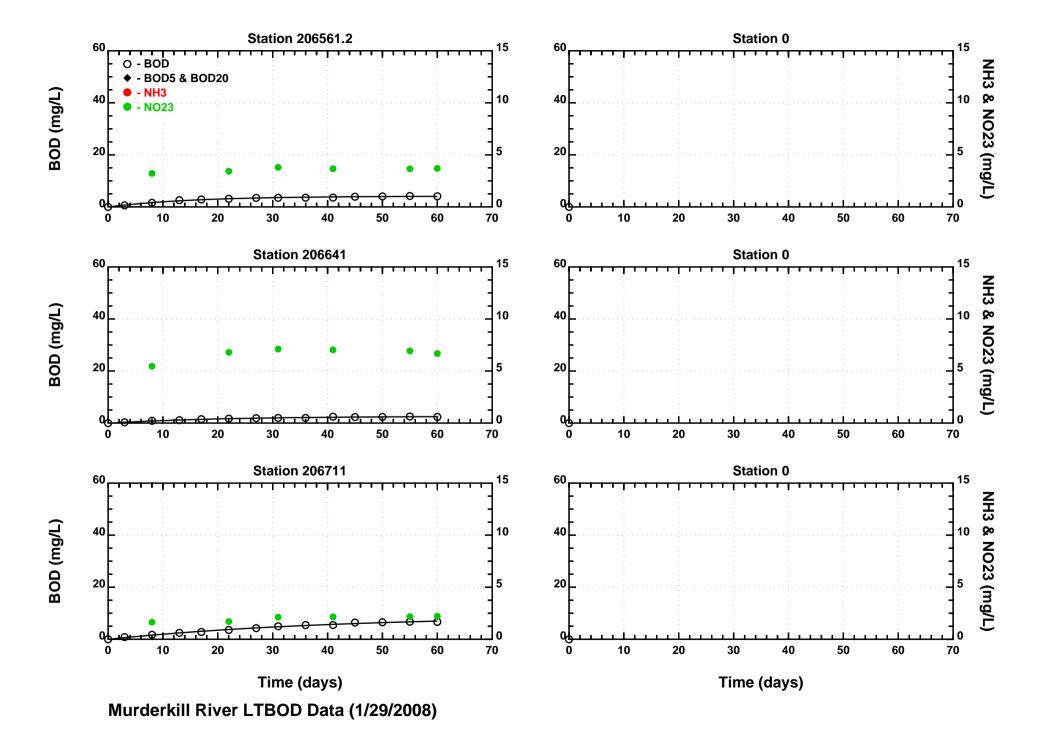


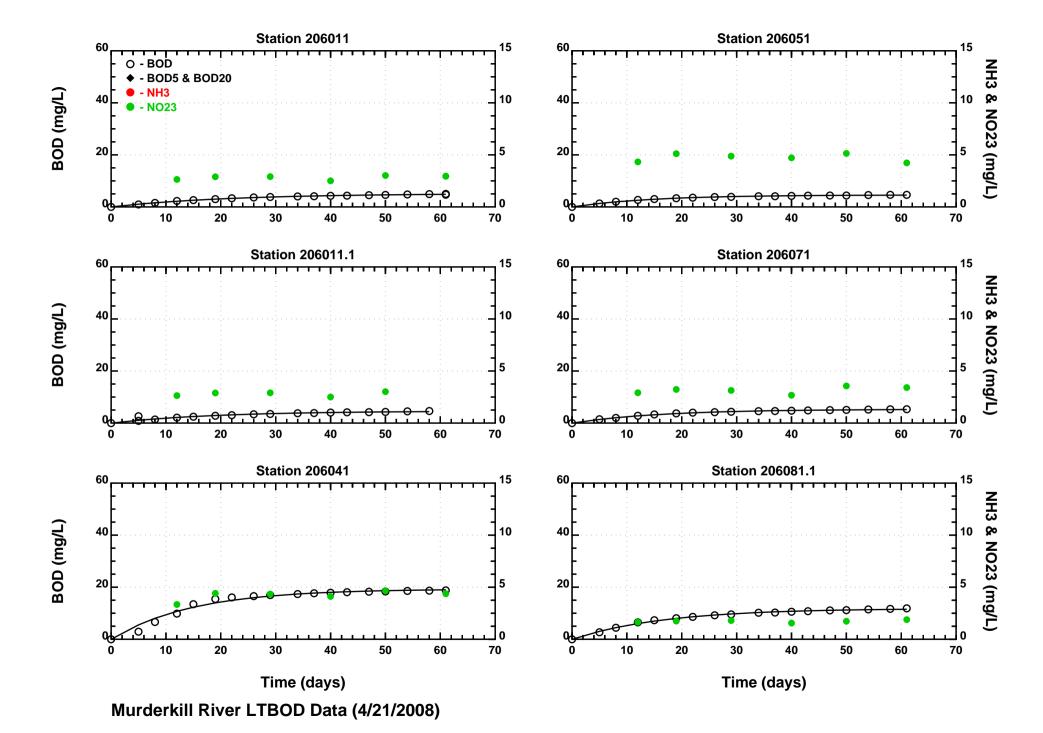


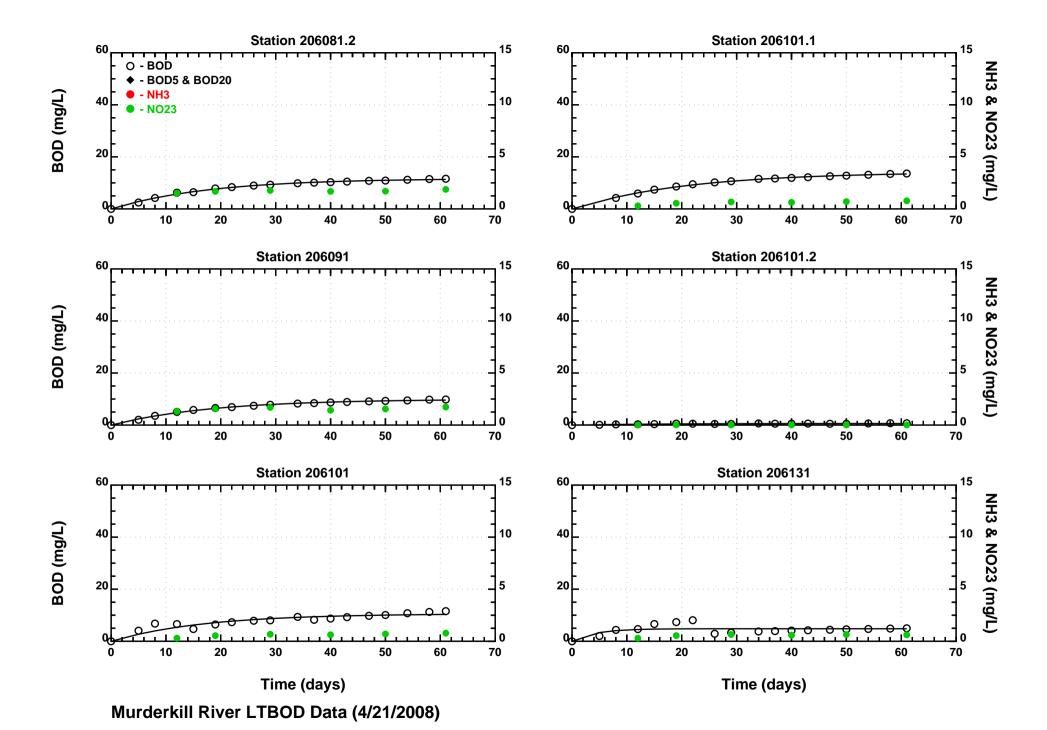


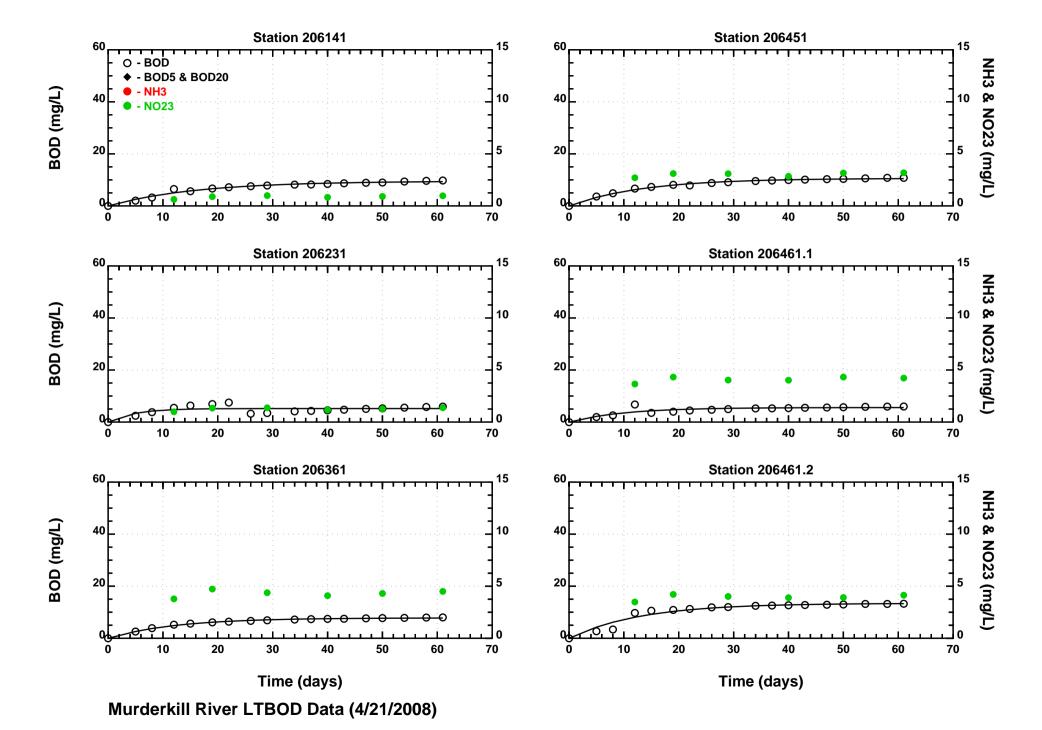


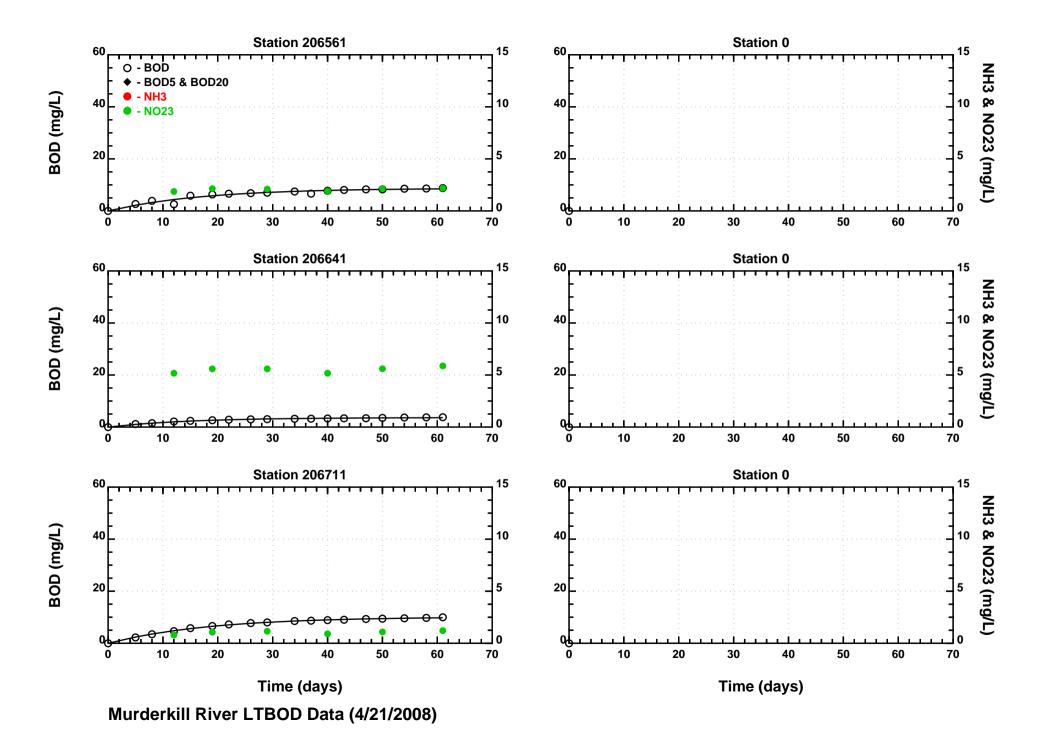


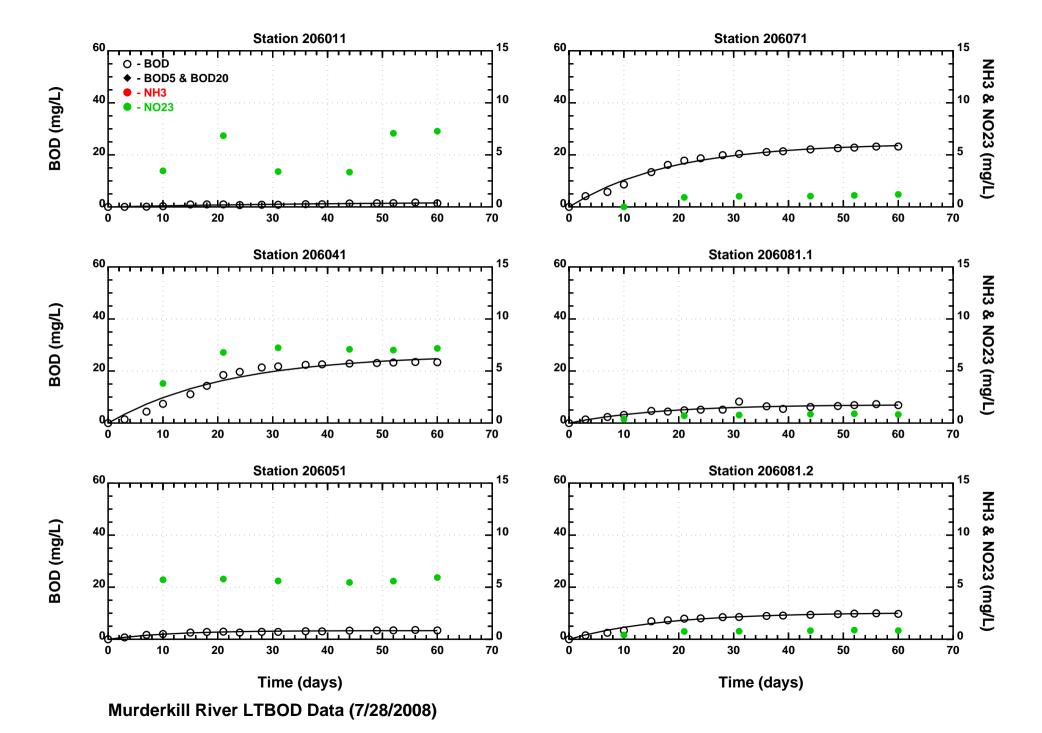


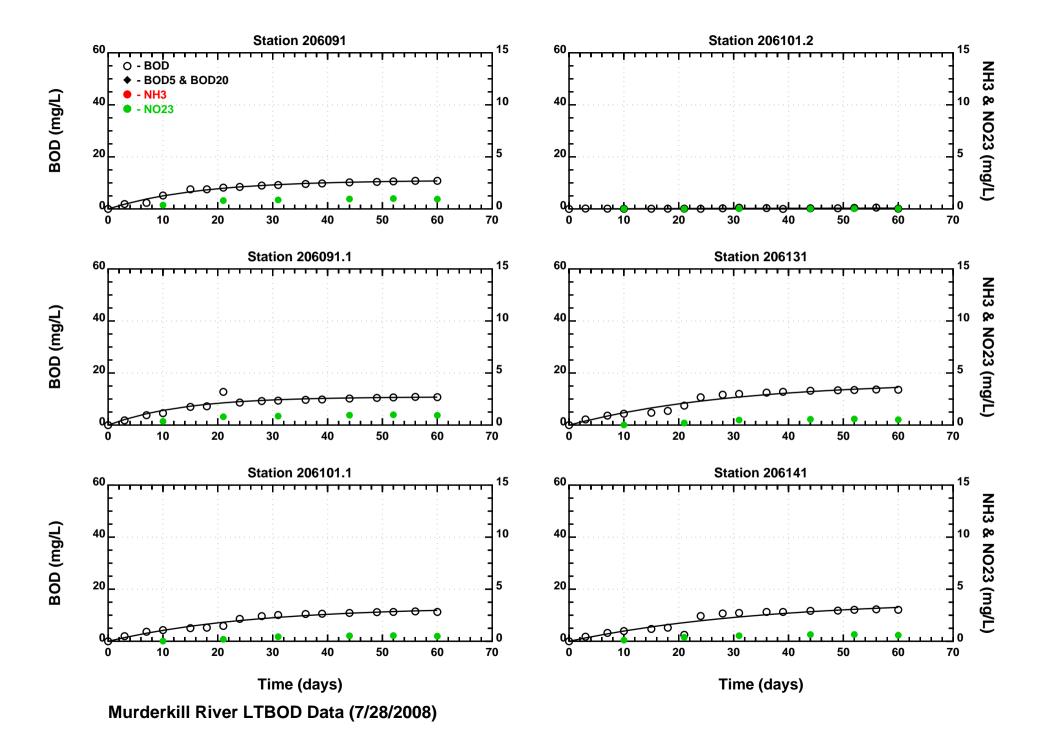


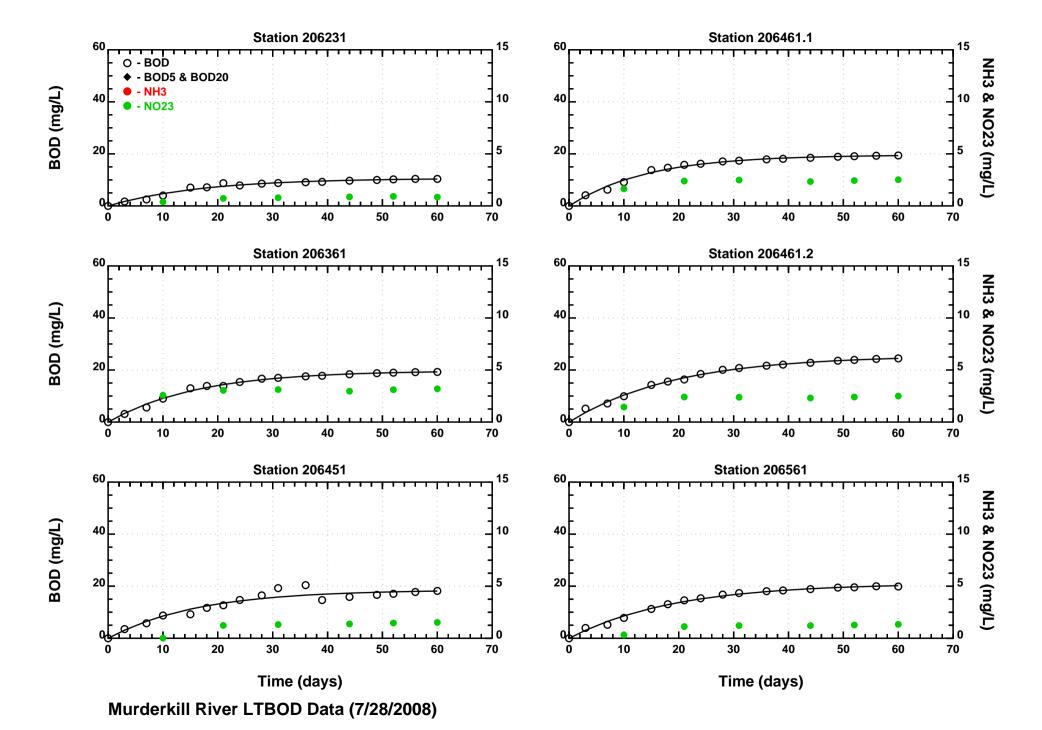


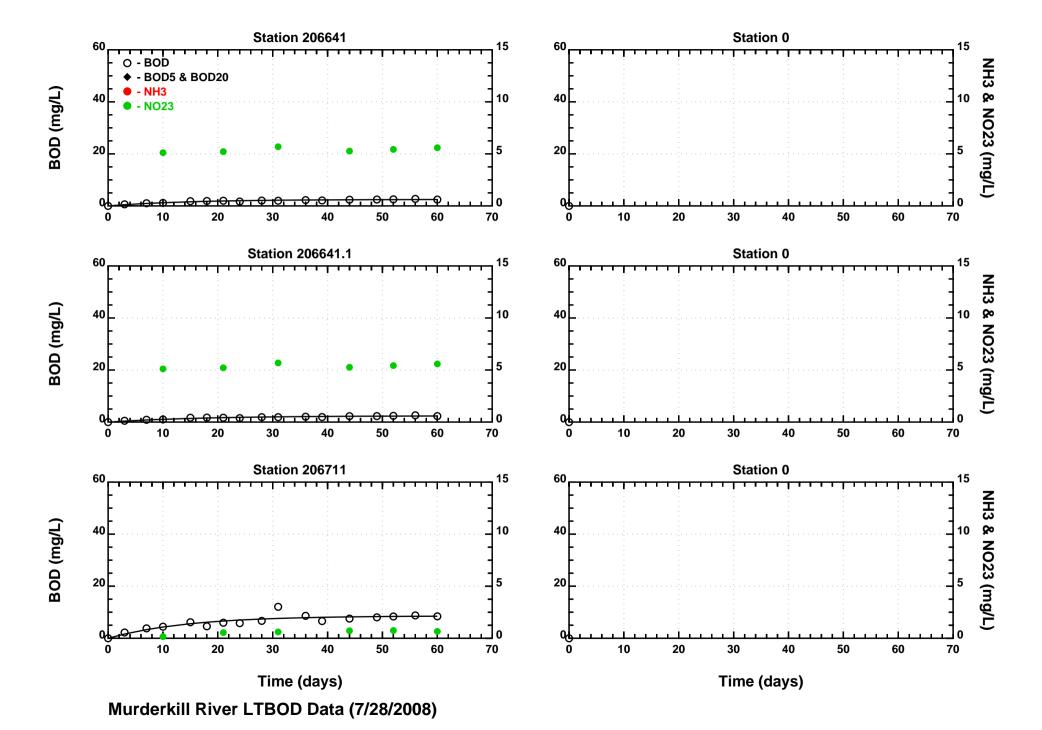






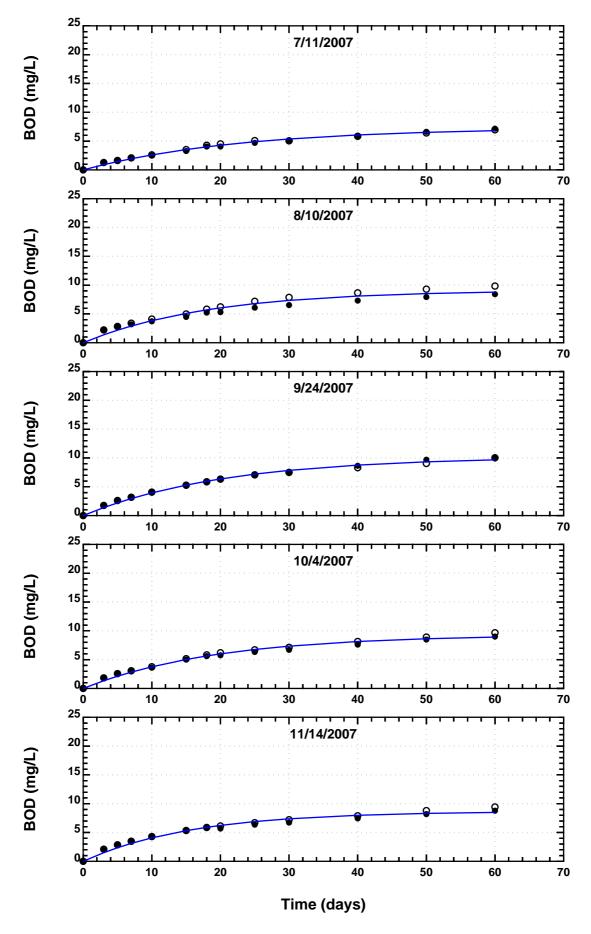




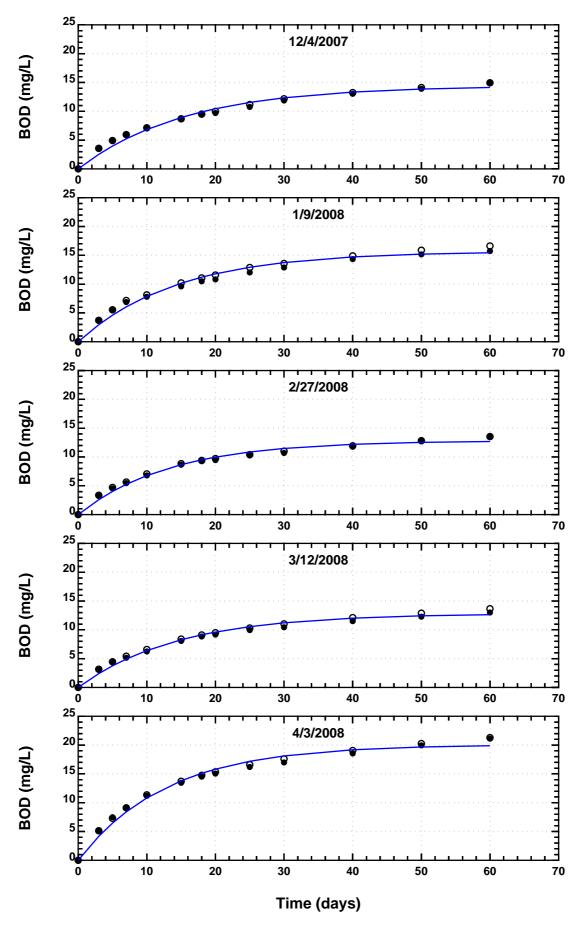


## **APPENDIX 9**

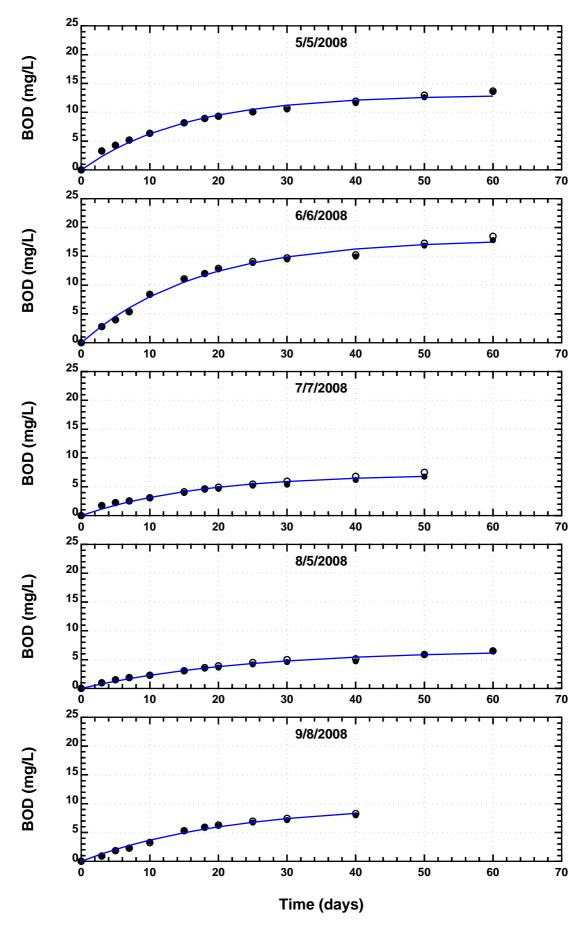
# LTBOD RESULTS FOR KCRWTF DISCHARGE



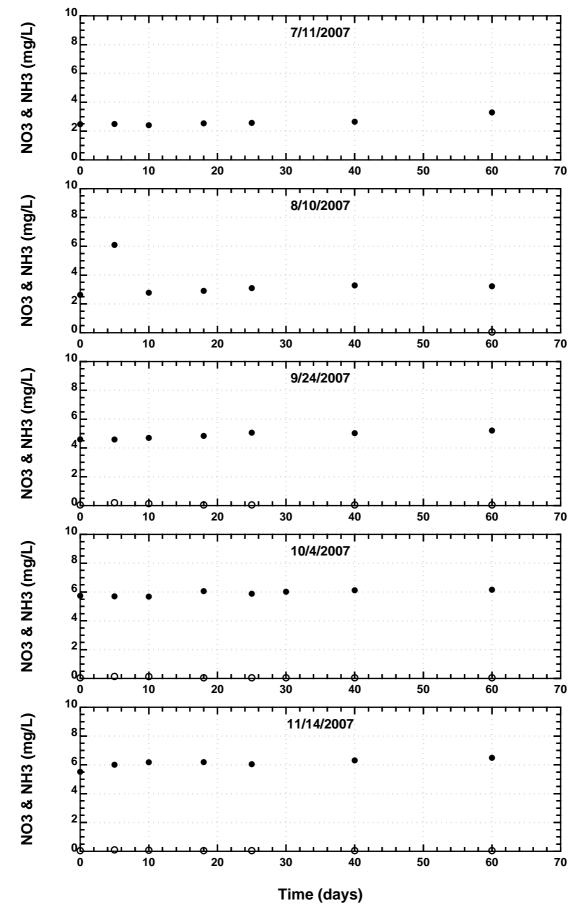
**Kent County WWTP Effluent LTBOD Data** 



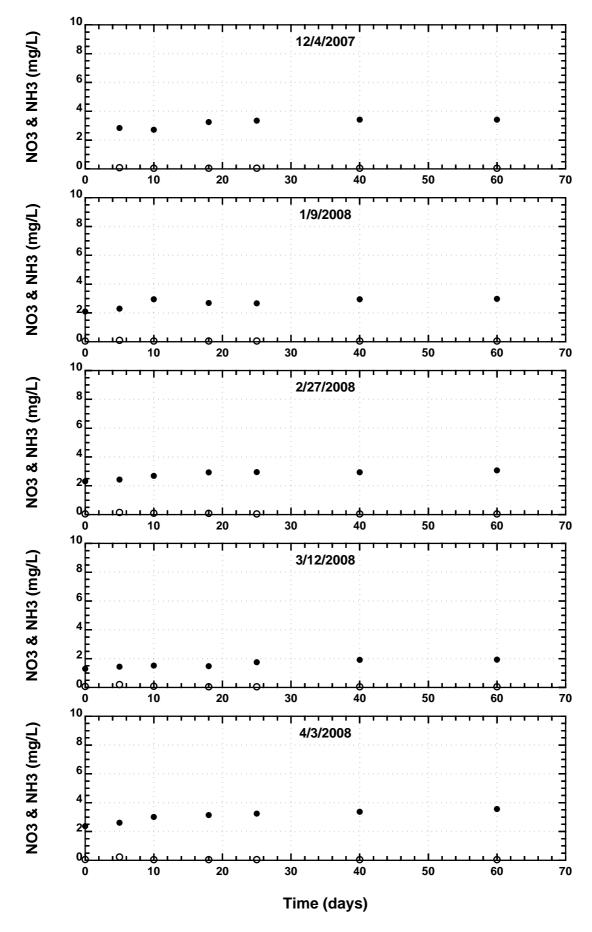
**Kent County WWTP Effluent LTBOD Data** 



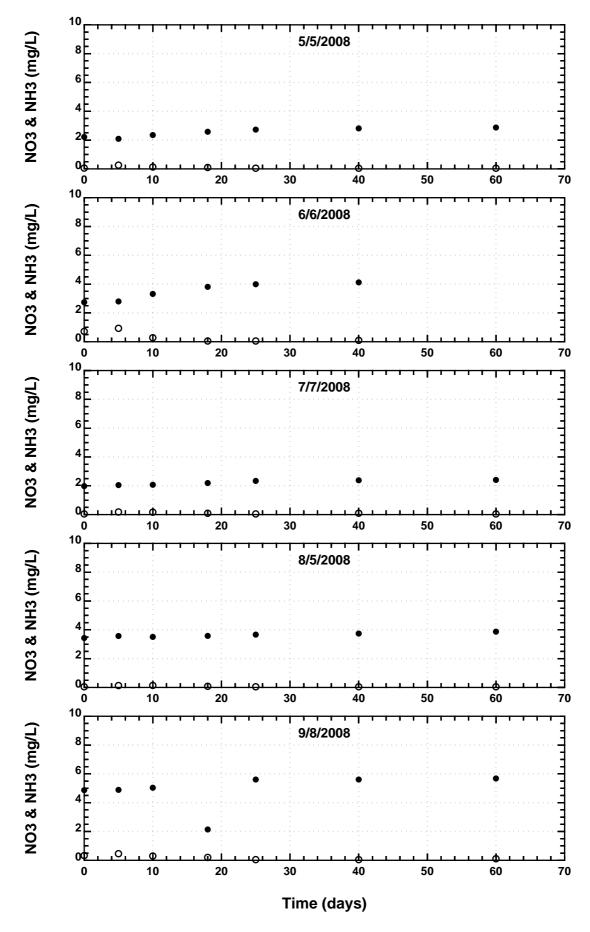
**Kent County WWTP Effluent LTBOD Data** 



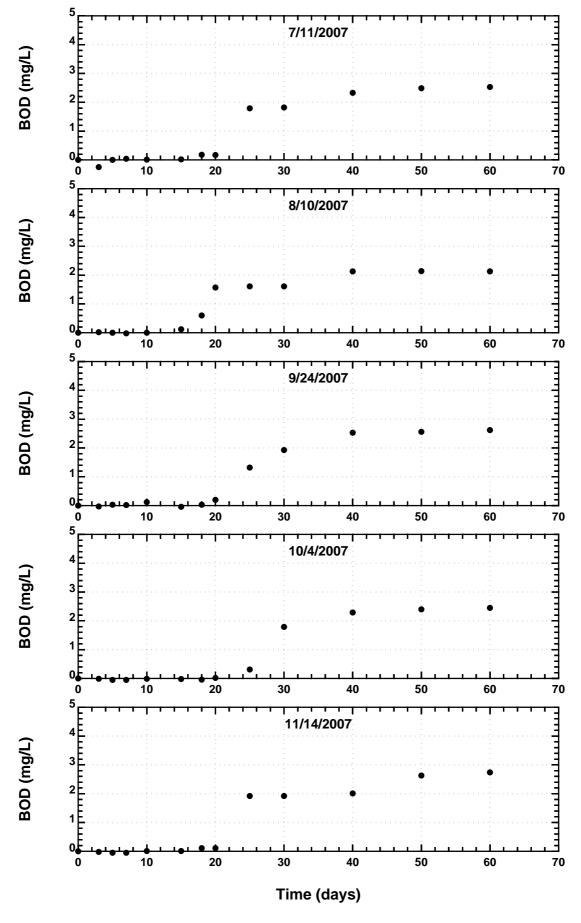
Kent County WWTP Effluent NO3 & NH3 Data



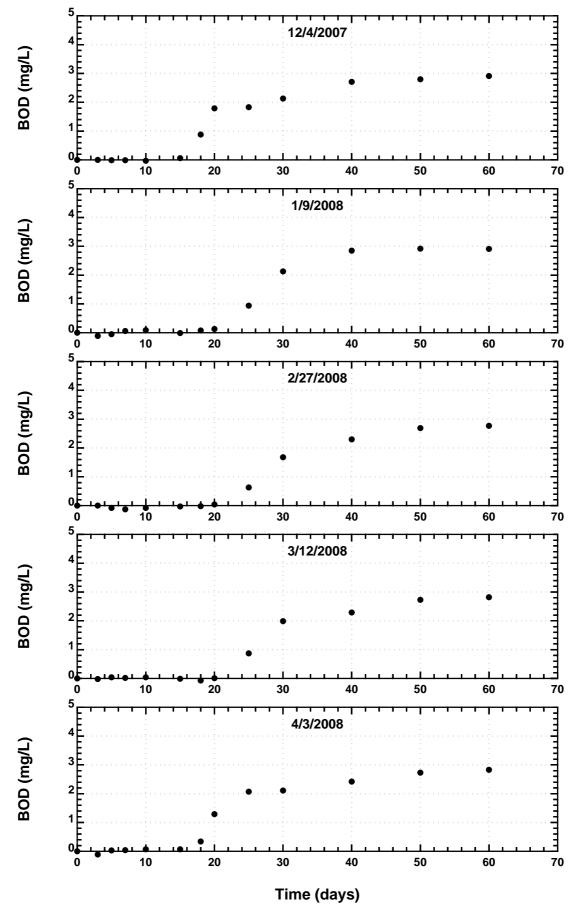
Kent County WWTP Effluent NO3 & NH3 Data



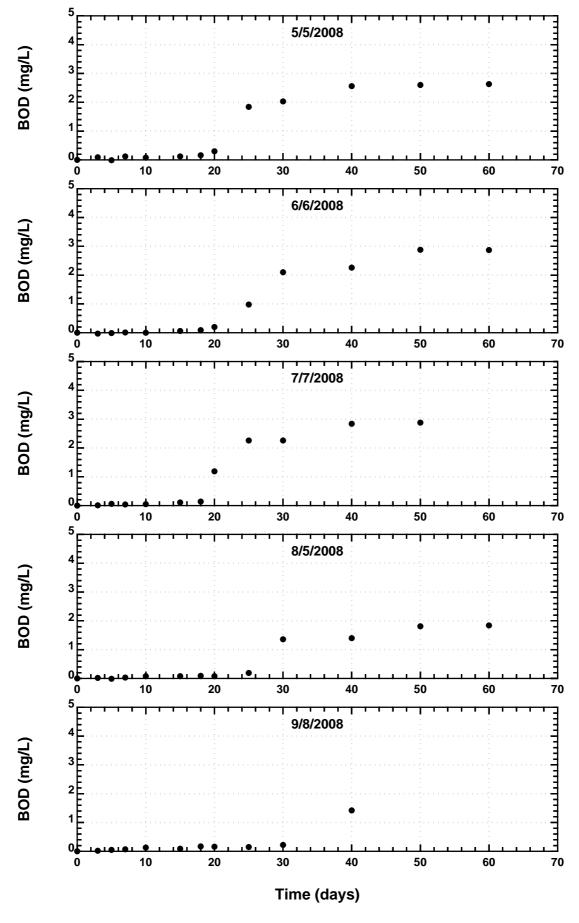
Kent County WWTP Effluent NO3 & NH3 Data



**Kent County WWTP Effluent LTBOD Data** 



**Kent County WWTP Effluent LTBOD Data** 



**Kent County WWTP Effluent LTBOD Data**